EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	2981	(("0000560") or ("0000126")).PN. or ((546/342) or (544/297) or (514/275) or (544/382) or (514/252.12)).CCLS.	US-PGPUB; USPAT	OR	OFF	2006/08/21 17:49
L2	1744	1 and chemical and compound	US-PGPUB; USPAT	OR	ON	2006/08/21 18:04
L3	0	1 and chemical and compound and hPPAR	US-PGPUB; USPAT	OR	ON	2006/08/21 18:04

8/21/06 6:13:47 PM

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chain nodes:

1 2 3 4 5 6 7 8 13 22 23 24 25 26 27 33 34 35 43 45

ring nodes:

16 17 18 19 20 21 36 37 38 39 40 41

chain bonds:

1-2 2-3 2-4 4-13 6-7 13-18 21-33 22-23 25-26 33-34 34-35 34-43

ring bonds:

16-17 16-21 17-18 18-19 19-20 20-21 36-37 36-41 37-38 38-39 39-40 40-41

exact/norm bonds:

4-13 13-18 21-33 25-26 33-34 34-35 34-43

exact bonds:

2-4 6-7 22-23

normalized bonds:

1-2 2-3 16-17 16-21 17-18 18-19 19-20 20-21 36-37 36-41 37-38 38-39 39-40 40-41

isolated ring systems:

containing 16: 36:

G1:[*1],[*2],[*3]

G2:[*4],[*5],[*6],[*7],[*8]

Match level:

1:CLASS2:CLASS3:CLASS4:CLASS5:CLASS6:CLASS7:CLASS8:CLASS13:CLASS16:Atom 17:Atom

18:Atom

19:Atom 20:Atom 21:Atom 22:CLAS\(23:CLAS\(24:CLAS\(25:CLAS\(26:CLAS\(27:CLAS\(33:CLAS\(34:CLAS\(35:CLAS\(34:CLAS\(34:CLAS\(35:CLAS\(34:CLA

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                 CA/CAplus enhanced with 1900-1906 U.S. patent records
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        MAY 19
                 Derwent World Patents Index to be reloaded and enhanced
                 IPC 8 Rolled-up Core codes added to CA/CAplus and
NEWS
        MAY 30
                 USPATFULL/USPAT2
        MAY 30
                 The F-Term thesaurus is now available in CA/CAplus
NEWS
NEWS 10
         JUN 02
                 The first reclassification of IPC codes now complete in
                 INPADOC
NEWS 11
         JUN 26
                 TULSA/TULSA2 reloaded and enhanced with new search and
                 and display fields
                 Price changes in full-text patent databases EPFULL and PCTFULL
NEWS 12
        JUN 28
                 CHEMSAFE reloaded and enhanced
NEWS 13
        JUl 11
                 FSTA enhanced with Japanese patents
NEWS 14
        JUl 14
NEWS 15
        JUl 19
                 Coverage of Research Disclosure reinstated in DWPI
                 INSPEC enhanced with 1898-1968 archive
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        AUG 09
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NEWS EXPRESS JUNE 30 CURRENT WINDOWS VERSION IS V8.01b, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 26 JUNE 2006.

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Updated Search

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SINCE FILE TOTAL ENTRY SESSION 0.42 0.42

FULL ESTIMATED COST

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STRUCTURE FILE UPDATES: 20 AUG 2006 HIGHEST RN 902860-89-3 DICTIONARY FILE UPDATES: 20 AUG 2006 HIGHEST RN 902860-89-3

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=> d 11

L1 HAS NO ANSWERS

L1 STR

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Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 14:03:19 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 37467 TO ITERATE

5.3% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01 0 ANSWERS

BEARCH TIME: 00:00:01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 737776 TO 760904
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 166.50 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y FULL SEARCH INITIATED 14:03:24 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 746924 TO ITERATE

99.2% PROCESSED 741084 ITERATIONS

197 ANSWERS

100.0% PROCESSED 746924 ITERATIONS

197 ANSWERS

SEARCH TIME: 00.00.17

L3 197 SEA SSS FUL L1

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=> file hcaplus
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 180.14 180.56

FULL ESTIMATED COST

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L4 26 L3

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L5 1 L4 AND BESWICK, P?/AU

=> d 15, ibib abs hitstr, 1

L5 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:

2004:2818 HCAPLUS

DOCUMENT NUMBER:

140:59406

TITLE:

Preparation of [[[(hetero)arylamino]methyl]phenoxy]ace tic acid derivatives as hPPAR activators for treatment

of cardiovascular disease and related disorders

INVENTOR(S):
Beswick, Paul John; Harling, John David;

Kleanthous, Savvas; Patel, Vipulkumar Kantibhai;

Simpson, Juliet

PATENT ASSIGNEE(S):

Smithkline Beecham Corporation, USA

SOURCE: PCT Int. Appl., 98 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

									APPLICATION NO.											
WO	WO 2004000762				A2 20031231			WO 2003-EP6416							20030618					
WO	WO 2004000762				A3 20041014															
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NO 2004005327							2005													
US 2006074111					A1		2006	0406												
PRIORITY APPLN. INFO.:																	0020			
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OTHER SOURCE(S):						PAT	140:	5940	6											

GI

HO
$$R^{1}$$
 R^{2} R^{3} R^{5} R^{5} R^{6} R^{4} R^{6}

Title compds. I [wherein R1 and R2 = independently H or alkyl; X = a bond, CH2, or O; R3 and R4 = independently H, alkyl, OCH3, CF3, allyl, or halo; X1 = CH2, SO2, or CO; R5 = alkenyl, alkanoyl, alkylsulfonyl, or (un)substituted alkyl(phenyl); R6 = (un)substituted Ph or 6-membered heteroaryl; or pharmaceutically acceptable salts, solvates, or hydrolyzable esters thereof] were prepared as human peroxisome proliferator activated receptor (hPPAR) activators. For example, coupling of Et 2-methyl-2-[2-methyl-4-[[[4-(trifluoromethyl)benzyl]amino]methyl]phenoxy]p ropanoate with 2-bromo-6-[4-(trifluoromethyl)phenyl]pyridine in the presence of Pd(OAc)2, (R)-2,2'-bis(diphenylphosphino)-1,1'-binaphthyl, and cesium carbonate in toluene gave the tertiary amine. Saponification with NaOH

in THF provided the acid II. Compds. of the invention showed at least 50% activation of hPPAR δ relative to the pos. control at concns. of 10-7 M or less. Thus, I and their pharmaceutical compns. are useful for the treatment of hPPAR mediated conditions, such as dyslipidemia, syndrome X, heart failure, hypercholesterolemia, cardiovascular disease, type II diabetes mellitus, type I diabetes, insulin resistance, hyperlipidemia, obesity, anorexia bulimia, or anorexia nervosa (no data). IT 637353-35-6P, [4-[[Butyl[4'-(trifluoromethyl)-1,1'-biphenyl-3yl]amino]methyl]-2-methylphenoxy]acetic acid 637353-36-7P, [4-[[(2-Methoxyethyl)[4'-(trifluoromethyl)-1,1'-biphenyl-3yl]amino]methyl]-2-methylphenoxy]acetic acid 637353-37-8P, [2-Methyl-4-[[(pentyl)[4'-(trifluoromethyl)-1,1'-biphenyl-3yl]amino]methyl]phenoxy]acetic acid 637353-38-9P, [4-[(2-Cyclopropylethyl)[4'-(trifluoromethyl)-1,1'-biphenyl-3yl]amino]methyl]-2-methylphenoxy]acetic acid 637353-39-0P, [2-Methyl-4-[[propyl[4'-(trifluoromethyl)-1,1'-biphenyl-3yl]amino]methyl]phenoxy]acetic acid 637353-40-3P, [2-Methyl-4-[[[2-(methylthio)ethyl][4'-(trifluoromethyl)-1,1'-biphenyl-3yl]amino]methyl]phenoxy]acetic acid 637353-41-4P, [4-[Butyl[2-methyl-4'-(trifluoromethyl)-1,1'-biphenyl-3-yl]amino]methyl]-2-methylphenoxy]acetic acid 637353-42-5P, [4-[[(2-Methoxyethyl) [2-methyl-4'-(trifluoromethyl)-1,1'-biphenyl-3yl]amino]methyl]-2-methylphenoxy]acetic acid 637353-43-6P,

[4-[[(Butyryl)[4'-(trifluoromethyl)-1,1'-biphenyl-3-yl]amino]methyl]-2-

methylphenoxy]acetic acid 637353-44-7P, [2-Methyl-4-

```
[[(propylsulfonyl)[4'-(trifluoromethyl)-1,1'-biphenyl-3-
yl]amino]methyl]phenoxy]acetic acid 637353-45-8P,
[4-[[Butyl[4'-(trifluoromethyl)-1,1'-biphenyl-3-yl]amino]sulfonyl]-2-
methylphenoxy]acetic acid 637353-46-9P, [2-Methyl-4-
[[(pentyl)[4'-(trifluoromethyl)-1,1'-biphenyl-3-
yl]amino]sulfonyl]phenoxy]acetic acid 637353-47-0P,
[4-[[(2-Cyclopropylethyl)[4'-(trifluoromethyl)-1,1'-biphenyl-3-
yl]amino]sulfonyl]-2-methylphenoxy]acetic acid 637353-56-1P,
[4-[Butyl(2,4'-dimethyl-1,1'-biphenyl-3-yl)amino]methyl]-2-
methylphenoxy]acetic acid 637353-57-2P, [4-[[Butyl(4'-fluoro-2-
methyl-1,1'-biphenyl-3-yl)amino]methyl]-2-methylphenoxy]acetic acid
637353-58-3P, [4-[[Butyl(4'-cyano-2-methyl-1,1'-biphenyl-3-
yl)amino]methyl]-2-methylphenoxy]acetic acid 637353-59-4P,
[4-[[Butyl(4'-methoxy-2-methyl-1,1'-biphenyl-3-yl)amino]methyl]-2-
methylphenoxy]acetic acid 637353-60-7P, [4-[[Butyl(4'-chloro-2-
methyl-1,1'-biphenyl-3-yl)amino]methyl]-2-methylphenoxy]acetic acid
637353-61-8P, [4-[(4'-Chloro-2-methyl-1,1'-biphenyl-3-yl)(2-
methoxyethyl)amino]methyl]-2-methylphenoxy]acetic acid
637353-62-9P, [4-[(2,4'-Dimethyl-1,1'-biphenyl-3-yl)(2-
methoxyethyl)amino]methyl]-2-methylphenoxy]acetic acid
637353-63-0P, [4-[[(2-Methoxyethyl)(4'-methoxy-2-methyl-1,1'-
biphenyl-3-yl)amino]methyl]-2-methylphenoxy]acetic acid
637353-64-1P, [2-Methyl-4-[[[2-methyl-4'-(trifluoromethyl)-1,1'-
biphenyl-3-yl](propyl)amino]methyl]phenoxy]acetic acid
637353-65-2P, [4-[[(4'-Chloro-2-methyl-1,1'-biphenyl-3-
yl) (propyl)amino]methyl]-2-methylphenoxy]acetic acid 637353-66-3P
, [4-[[(2,4'-Dimethyl-1,1'-biphenyl-3-yl)(propyl)amino]methyl]-2-
methylphenoxy]acetic acid 637353-67-4P, [4-[[(4'-Fluoro-2-methyl-
1,1'-biphenyl-3-yl)(propyl)amino]methyl]-2-methylphenoxy]acetic acid
637353-68-5P, [4-[[(4'-Cyano-2-methyl-1,1'-biphenyl-3-
yl)(propyl)amino]methyl]-2-methylphenoxy]acetic acid 637353-69-6P
, [4-[[(4'-Methoxy-2-methyl-1,1'-biphenyl-3-yl)(propyl)amino]methyl]-2-
methylphenoxy]acetic acid 637353-84-5P, [4-[[Butyl[2-methyl-4'-
(trifluoromethyl) -1,1'-biphenyl-3-yl]amino]sulfonyl]-2-
methylphenoxy]acetic acid
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
   (hPPAR activator; preparation of [[[(hetero)arylamino]methyl]phenoxy]acetic
   acid derivs. as hPPAR activators for treatment of cardiovascular
   disease and related disorders)
637353-35-6 HCAPLUS
Acetic acid, [4-[[butyl[4'-(trifluoromethyl)[1,1'-biphenyl]-3-
yl]amino]methyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)
```

```
RN 637353-36-7 HCAPLUS
CN Acetic acid, [4-[(2-methoxyethyl)[4'-(trifluoromethyl)[1,1'-biphenyl]-3-
yl]amino]methyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)
```

RN

CN

$$\begin{array}{c} \text{CH}_2-\text{CH}_2-\text{OMe} \\ \\ \text{N-R} \end{array}$$

$$\begin{array}{c} \text{Me} \\ \text{O-CH}_2\text{-CO}_2\text{H} \\ \text{R-CH}_2 \end{array}$$

RN 637353-37-8 HCAPLUS

CN Acetic acid, [2-methyl-4-[[pentyl[4'-(trifluoromethyl)[1,1'-biphenyl]-3-yl]amino]methyl]phenoxy]- (9CI) (CA INDEX NAME)

RN 637353-38-9 HCAPLUS

CN Acetic acid, [4-[[(2-cyclopropylethyl) [4'-(trifluoromethyl) [1,1'-biphenyl]-3-yl]amino]methyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

$$CH_2$$
 CH_2
 CH_2

RN 637353-39-0 HCAPLUS

CN Acetic acid, [2-methyl-4-[[propyl[4'-(trifluoromethyl)[1,1'-biphenyl]-3-yl]amino]methyl]phenoxy]- (9CI) (CA INDEX NAME)

RN 637353-40-3 HCAPLUS

CN Acetic acid, [2-methyl-4-[[[2-(methylthio)ethyl][4'-(trifluoromethyl)[1,1'-biphenyl]-3-yl]amino]methyl]phenoxy]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{F}_3\text{C} & \text{CH}_2\text{--}\text{CH}_2\text{--}\text{SMe} \\ \hline & \text{N}\text{---}\text{R} \end{array}$$

RN 637353-41-4 HCAPLUS

CN Acetic acid, [4-[[butyl[2-methyl-4'-(trifluoromethyl)[1,1'-biphenyl]-3-yl]amino]methyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

RN 637353-42-5 HCAPLUS

CN Acetic acid, [4-[[(2-methoxyethyl)[2-methyl-4'-(trifluoromethyl)[1,1'-biphenyl]-3-yl]amino]methyl]-2-methylphenoxyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{F}_3\text{C} & \text{Me} & \text{CH}_2\text{--}\text{CH}_2\text{--}\text{OMe} \\ \hline & \text{N}\text{---}\text{R} \\ \end{array}$$

$$\begin{array}{c} \text{Me} \\ \\ \text{O-CH}_2\text{-CO}_2\text{H} \\ \\ \\ \text{R-CH}_2 \end{array}$$

RN 637353-43-6 HCAPLUS

CN Acetic acid, [2-methyl-4-[[(1-oxobutyl)[4'-(trifluoromethyl)[1,1'-biphenyl]-3-yl]amino]methyl]phenoxy]- (9CI) (CA INDEX NAME)

RN 637353-44-7 HCAPLUS

CN Acetic acid, [2-methyl-4-[[(propylsulfonyl)[4'-(trifluoromethyl)[1,1'-biphenyl]-3-yl]amino]methyl]phenoxy]- (9CI) (CA INDEX NAME)

RN 637353-45-8 HCAPLUS

CN Acetic acid, [4-[[butyl[4'-(trifluoromethyl)[1,1'-biphenyl]-3-yl]amino]sulfonyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

RN 637353-46-9 HCAPLUS

CN Acetic acid, [2-methyl-4-[[pentyl[4'-(trifluoromethyl)[1,1'-biphenyl]-3-yl]amino]sulfonyl]phenoxy]- (9CI) (CA INDEX NAME)

$$CH_2)_4-Me$$
 $O=S=0$
 Me
 $O-CH_2-CO_2H$

RN 637353-47-0 HCAPLUS

CN Acetic acid, [4-[[(2-cyclopropylethyl) [4'-(trifluoromethyl) [1,1'-biphenyl]-3-yl]amino]sulfonyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

$$HO_2C-CH_2-O$$
 Me
 $O=S=O$
 CH_2-CH_2-N
 CF_3

RN 637353-56-1 HCAPLUS

CN Acetic acid, [4-[[butyl(2,4'-dimethyl[1,1'-biphenyl]-3-yl)amino]methyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

Me N-Bu
$$O-CH_2-CO_2H$$

RN 637353-57-2 HCAPLUS

CN Acetic acid, [4-[[butyl(4'-fluoro-2-methyl[1,1'-biphenyl]-3-yl)amino]methyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{N-Bu} & \text{O-CH}_2\text{-CO}_2\text{H} \\ \hline \\ \text{N-CH}_2 & \text{O-CH}_2\text{-CO}_2\text{H} \\ \end{array}$$

RN 637353-58-3 HCAPLUS

CN Acetic acid, [4-[[butyl(4'-cyano-2-methyl[1,1'-biphenyl]-3-yl)amino]methyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

NC Me
$$n-Bu$$
 $O-CH_2-CO_2H$

RN 637353-59-4 HCAPLUS

CN Acetic acid, [4-[[butyl(4'-methoxy-2-methyl[1,1'-biphenyl]-3-yl)amino]methyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

MeO Me
$$n-Bu$$
 $O-CH_2-CO_2H$

RN 637353-60-7 HCAPLUS

CN Acetic acid, [4-[[butyl(4'-chloro-2-methyl[1,1'-biphenyl]-3-yl)amino]methyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

RN 637353-61-8 HCAPLUS

CN Acetic acid, [4-[[(4'-chloro-2-methyl[1,1'-biphenyl]-3-yl)(2-methoxyethyl)amino]methyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{C1} & \text{Me} & \text{CH}_2\text{--}\text{CH}_2\text{--}\text{OMe} \\ & \text{N} & \text{R} \end{array}$$

RN 637353-62-9 HCAPLUS

CN Acetic acid, [4-[[(2,4'-dimethyl[1,1'-biphenyl]-3-yl)(2-methoxyethyl)amino]methyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{CH}_2-\text{CH}_2-\text{OMe} \\ \hline & \text{N--R} \end{array}$$

RN 637353-63-0 HCAPLUS

CN Acetic acid, [4-[[(2-methoxyethyl)(4'-methoxy-2-methyl[1,1'-biphenyl]-3-yl)amino]methyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{MeO} & \text{Me} \\ \text{CH}_2\text{--}\text{CH}_2\text{--}\text{OMe} \\ \text{N---}\text{R} \end{array}$$

$$\begin{array}{c} \text{Me} \\ \text{O-CH}_2\text{-CO}_2\text{H} \\ \\ \text{R-CH}_2 \end{array}$$

RN 637353-64-1 HCAPLUS

CN Acetic acid, [2-methyl-4-[[[2-methyl-4'-(trifluoromethyl)[1,1'-biphenyl]-3-yl]propylamino]methyl]phenoxy]- (9CI) (CA INDEX NAME)

RN 637353-65-2 HCAPLUS

CN Acetic acid, [4-[[(4'-chloro-2-methyl[1,1'-biphenyl]-3-yl)propylamino]methyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

C1 Me
$$n-Pr$$
 $N-CH_2$ $O-CH_2-CO_2H$

RN 637353-66-3 HCAPLUS

CN Acetic acid, [4-[[(2,4'-dimethyl[1,1'-biphenyl]-3-yl)propylamino]methyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

Me
$$n-Pr$$
 $N-CH_2$ $O-CH_2-CO_2H$

RN 637353-67-4 HCAPLUS

CN Acetic acid, [4-[[(4'-fluoro-2-methyl[1,1'-biphenyl]-3-yl)propylamino]methyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} & \text{N-Pr} \\ \hline & \text{N-CH}_2 & \text{O-CH}_2\text{--}\text{CO}_2\text{H} \\ \hline \end{array}$$

RN 637353-68-5 HCAPLUS

CN Acetic acid, [4-[[(4'-cyano-2-methyl[1,1'-biphenyl]-3-yl)propylamino]methyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{NC} & \text{Me} & \text{O-CH}_2\text{--CO}_2\text{H} \\ \hline & \text{N-CH}_2 & \text{O-CH}_2\text{--CO}_2\text{H} \\ \end{array}$$

MeO Me
$$n-Pr$$
 $N-CH_2$ $O-CH_2-CO_2H$

RN 637353-84-5 HCAPLUS
CN Acetic acid, [4-[[butyl[2-methyl-4'-(trifluoromethyl)[1,1'-biphenyl]-3yl]amino]sulfonyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

$$F_3C$$
 $N-S$
 $O-CH_2-CO_2H$

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FILE 'REGISTRY' ENTERED AT 13:45:23 ON 21 AUG 2006

STRUCTURE UPLOADED

L2 0 S L1

L3 197 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 14:03:46 ON 21 AUG 2006

L4 26 S L3

L5 1 S L4 AND BESWICK, P?/AU

=> s 14 not 15

L6 25 L4 NOT L5

=> s 16 and harling, j?/au

66 HARLING, J?/AU

L7 0 L6 AND HARLING, J?/AU

```
=> s 16 and kleanthous, s?/au
            11 KLEANTHOUS, S?/AU
             0 L6 AND KLEANTHOUS, S?/AU
L8
=> s 16 and lambert, m?/au
           961 LAMBERT, M?/AU
             0 L6 AND LAMBERT, M?/AU
L9
=> s 16 and kantibhai, v?/au
             0 KANTIBHAI, V?/AU
L10
             0 L6 AND KANTIBHAI, V?/AU
=> s 16 and simpson, j?/au
          2346 SIMPSON, J?/AU
L11
             0 L6 AND SIMPSON, J?/AU
=> d his
     (FILE 'HOME' ENTERED AT 13:44:31 ON 21 AUG 2006)
     FILE 'REGISTRY' ENTERED AT 13:45:23 ON 21 AUG 2006
               STRUCTURE UPLOADED
L1
              0 S L1
L2
            197 S L1 FULL
L3
     FILE 'HCAPLUS' ENTERED AT 14:03:46 ON 21 AUG 2006
L4
             26 S L3
             1 S L4 AND BESWICK, P?/AU
L5
             25 S L4 NOT L5
L6
             0 S L6 AND HARLING, J?/AU
L7
             0 S L6 AND KLEANTHOUS, S?/AU
L8
L9
              0 S L6 AND LAMBERT, M?/AU
L10
              0 S L6 AND KANTIBHAI, V?/AU
              0 S L6 AND SIMPSON, J?/AU
L11
=> d 14, ibib abs hitstr, 1-25
     ANSWER 1 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER:
                     2006:655920 HCAPLUS
DOCUMENT NUMBER:
                         145:124613
                         Preparation of carboxylic acid derivatives having
TITLE:
                         three cyclic moieties as anticoagulants
INVENTOR(S):
                         Ishihara, Tsukasa; Miura, Masanori; Ohne, Kazuhiko;
                         Takuwa, Tomofumi; Shirakami, Shohei; Ibuka, Ryotaro;
                         Ohnuki, Kei; Seki, Norio; Shigenaga, Takeshi;
                         Hirayama, Fukushi; Hirabayashi, Akihito; Kai,
                         Yuichiro; Kobayashi, Junichi; Hirasawa, Hideaki;
                         Kondou, Atsushi; Yamada, Ken
PATENT ASSIGNEE(S):
                         Astellas Pharma Inc., Japan
SOURCE:
                         PCT Int. Appl., 198 pp.
                         CODEN: PIXXD2
DOCUMENT TYPE:
                         Patent
LANGUAGE:
                         Japanese
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
     PATENT NO.
                         KIND
                              DATE
                                          APPLICATION NO.
                                                                  DATE
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GΙ

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20060706
     WO 2006070878
                                            WO 2005-JP24096
                                                                   20051228
                          A1
            AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR,
             KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX,
             MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE,
             SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC,
             VN, YU, ZA, ZM, ZW
         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
             CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
             GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM
                                            JP 2004-380131
PRIORITY APPLN. INFO.:
                                                                A 20041228
```

$$(R^{4})_{p} \xrightarrow{C} X - Y \xrightarrow{0} R^{5}$$

$$\downarrow L \\ (R^{2})_{m} A \xrightarrow{J} B \xrightarrow{R^{3}} (R^{3})_{n}$$

The title compds. [I; ring A = aryl or heteroaryl ring; ring B = benzene, AB naphthalene, or monocyclic or bicyclic heteroaryl ring; ring C = cycloalkyl, aryl, or heterocyclic ring; m, n, p = an integer of 0-3; R1 = NH2, CH2NH2, CONH2, C(:NH)NH2, C(:NOH)NH2, C(:NH)NH-CO2-(optionally substituted lower alkyl), 5-oxo-2,5-dihydro-1,2,4-oxadiazol-3-yl; R2, R3 = lower alkyl, halo-lower alkyl, halo, oxo, cyano, NO2, halo-lower alkoxy, NROROO, SRO, S(O)RO, SO2RO, SO2NROROO, NROSO2ROO, CORO, CO2RO, CONROROO, NROCOR00, NROCO-(halo-lower alkyl), cycloalkyl, aryl, heterocyclyl, etc.; R0, R00 = H, lower alkyl; R4 = lower alkyl, lower alkenyl, cycloalkyl, aryl, heterocyclyl, halo, oxo, cyano, NO2, OR6, NR6R6a, SR6, SOR6, SO2R6, SO2NR6R6a, NR6SO2R6a, NR6SO2NR6R6a, NR6SO2NR6aCO2R6a, COR6, CO2R6, CONR6R6a, cycloalkyl, aryl, heterocyclyl, etc.; R6, R6a = H, each (un) substituted lower alkyl, lower alkenyl, cycloalkyl, aryl, or heterocyclyl; R5 = OR0, NR0R00, N(R0)-lower alkylene-OR00; J = NR0CO, CONRO, NROCONRO, NRO-lower alkylene, lower alkylene-NROCO; L = NRO-lower alkylene, NRO-lower alkenylene, lower alkylene, lower alkenylene; X = a single bond, (un) substituted NH, S, CO, SO, SO2, lower alkylene-O, lower alkylene-(un)substituted NH; Y = a single bond, each (un)substituted lower alkylene or lower alkenylene] or pharmaceutically acceptable salt thereof are prepared These compds. such as phenoxyacetic acid and phenylpropanoic acid derivs. or salts thereof have an anticoagulant effect based on the inhibition of the activated blood coagulation factor VII and, therefore, are useful as blood coagulation inhibitors or preventives/remedies for diseases caused by thrombus or embolus. They are also selective inhibitors of activated blood coagulation factor VII over activated blood coagulation factor X and thrombin. The above diseases include ischemic heart diseases, restenosis after angioplasty, cerebral thrombosis, transient cerebral ischemia, peripheral arterial obstruction, Charcot's syndrome (intermittent claudication), deep venous thrombosis, pulmonary embolism, disseminated intravascular coagulation (DIC), thrombogenesis

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RN

after heart valve replacement surgery, coagulation or inflammation of circulating blood during external blood circulation, arteriosclerosis, and cancer. For example, [(3-([(2-([(2-amino-1H-benzimidazol-5-yl)amino]carbonyl)-4-chlorophenyl)amino]methyl)biphenyl-2-yl)oxy]acetic acid in vitro inhibited activated blood coagulation factor VII over activated blood coagulation factor X and thrombin with IC50 of 0.36, ≥ 100 , and $\geq 100~\mu M$, resp.

IT 897632-55-2P, [2-[[[4-[Amino(imino)methyl]phenyl]amino]carbon yl]-4-chlorophenyl]amino]methyl]-4-[(dimethylamino)methyl]-6-ethoxyphenoxy]acetic acid hydrochloride 897635-46-0P 897635-49-3P 897636-55-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of carboxylic acid derivs. having three cyclic moieties as activated blood coagulation factor VII inhibitors and anticoagulants) 897632-55-2 HCAPLUS

CN INDEX NAME NOT YET ASSIGNED

C1
$$C-NH_2$$
 $C-NH_2$ CH_2-NMe_2 CH_2-NMe_2 CH_2-NMe_2 CH_2-NMe_2

●x HCl

RN 897635-46-0 HCAPLUS CN INDEX NAME NOT YET ASSIGNED

CM 1

CRN 897635-45-9 CMF C30 H36 Cl N5 O5

C1
$$C-NH_2$$
 $C-NH_2$ $CH_2-N-Pr-i$ $CH_2-N-Pr-i$ $CH_2-N-Pr-i$ $CH_2-N-Pr-i$ $CH_2-N-Pr-i$

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 897635-49-3 HCAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} & \text{NH} \\ & \text{C-NH}_2 \\ & \text{C-NH}_2 \\ & \text{NH-CH}_2 \\ & \text{HO}_2\text{C-CH}_2\text{-O} \\ & \text{OEt} \end{array}$$

●x HCl

RN 897636-55-4 HCAPLUS CN INDEX NAME NOT YET ASSIGNED

CM 1

CRN 897636-54-3 CMF C29 H34 Cl N5 O5

C1
$$C-NH_2$$
 $C-NH_2$ $C-NH_2$ CH_2-NMe_2 CH_2-NMe_2 CH_2-NMe_2 CH_2-NMe_2

CM 2

CRN 64-18-6 CMF C H2 O2

O== CH- OH

REFERENCE COUNT:

32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 2 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN L4

ACCESSION NUMBER:

2006:117042 HCAPLUS

DOCUMENT NUMBER:

144:212778

TITLE:

Preparation of pyrazole derivatives and other

heterocyclic compounds as peroxisome proliferator-activated receptor α and γ

agonists

INVENTOR(S):

Kagechika, Katsuji; Yamaguchi, Mitsuhiro; Shibata,

Yoshihiro; Usui, Hiroyuki

PATENT ASSIGNEE(S):

Daiichi Pharmaceutical Co., Ltd., Japan

PCT Int. Appl., 186 pp.

SOURCE:

CODEN: PIXXD2

DOCUMENT TYPE: LANGUAGE:

GΙ

Patent Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATEN	PATENT NO.					DATE			APPL	ICAT:		DATE					
WO 20	WO 2006013939				A1 20060209			1	WO 2	005-		20050804					
W	: AE,	AG,	AL,	AM,	ΑT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BW,	BY,	ΒZ,	CA,	CH,	
	CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,	
	GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KM,	KP,	KR,	KZ,	
	LC, LK, LR,			LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	
	NG, NI, NO,				OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	
	SL,	SM,	SY,	ТJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UΖ,	VC,	VN,	YU,	
	ZA, ZM, ZW																
R	W: AT,	BE,	ВG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,	
	IS,	IT,	LT,	LU,	LV,	MC,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	BF,	ВJ,	
	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	ΝE,	SN,	TD,	TG,	BW,	GH,	
	GM,	KE,	LS,	MW,	ΜZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	ΑZ,	BY,	
	KG,	ΚZ,	MD,	RU,	ТJ,	TM											
PRIORITY APPLN. INFO.:					JP 2004-229445							i	A 20040805				
OTHER SOURCE(S):					MARPAT 144:212778												

$$\begin{array}{c|c}
(R6) m & R2 \\
X - Y & Q \\
R1 - N A & CH2) n & Q
\end{array}$$

$$\begin{array}{c|c}
R3 & R4 \\
OR5
\end{array}$$

The title compds. I [ring A = 5-member aromatic heterocyclic ring; X, Y, Z = AB

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Updated Search

N, C; m = 0 - 3; n = 1 - 5; Q = (un) substituted benzene ring; R1 = 1(un) substituted Ph, naphthyl, 5- or 6-member aromatic ring; R2 = (un) substituted alkyl, (un) substituted carbamoyl, (un) substituted Ph, etc.; R3, R4 = H, alkyl; R5 = H, alkyl, (un)substituted benzyl; R6 = H, OH, halo, etc.; when $m = \geq 2$, the R6 substituents may be the same or different] are prepared Thus, 2-[4-[[[1-(4-chlorophenyl)-3-methyl-1Hpyrazol-4-ylmethyl] furan-2-ylmethylamino] methyl] phenoxy] -2-methylpropionic acid was prepared in 2 steps from 4-chloromethyl-1-(4-chlorophenyl)-3-methyl-1H-pyrazole and 2-[4-[[(furan-2-ylmethyl)amino]methyl]phenoxy]-2methylpropionic acid Et ester. In GAL4-hPPAR transactivation assays (PPAR α), compds. of this invention showed EC50 values of 0.0028 μM to 0.08 μΜ. IT 875656-84-1P 875656-86-3P 875656-87-4P 875656-96-5P 875656-98-7P 875657-01-5P 875657-02-6P 875657-03-7P 875657-04-8P 875657-05-9P 875657-06-0P 875657-07-1P 875657-08-2P 875657-09-3P 875657-10-6P 875657-11-7P 875657-12-8P 875657-13-9P 875657-14-0P 875657-15-1P 875657-16-2P 875657-17-3P 875657-18-4P 875657-19-5P 875657-20-8P 875657-21-9P 875657-22-0P 875657-23-1P 875657-24-2P 875657-25-3P 875657-26-4P 875657-27-5P 875657-28-6P 875657-29-7P 875657-30-0P 875657-31-1P 875657-32-2P 875657-33-3P 875657-34-4P 875657-35-5P 875657-36-6P 875657-37-7P 875657-38-8P 875657-39-9P 875657-40-2P 875657-41-3P RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (preparation of pyrazole derivs. and other heterocyclic compds. as peroxisome proliferator-activated receptor α and γ agonists) RN 875656-84-1 HCAPLUS Propanoic acid, 2-[4-[[(2-furanylmethyl)]((3-methyl-1-phenyl-1H-pyrazol-4-CN y1) methy1]amino] methy1]-2,6-dimethy1phenoxy]-2-methy1- (9CI) (CA INDEX

RN 875656-86-3 HCAPLUS

NAME)

CN Propanoic acid, 2-[4-[[(2-furanylmethyl)](5-methyl-2-phenyl-2H-1,2,3-triazol-4-yl)methyl]amino]methyl]-2,6-dimethylphenoxy]-2-methyl- (9CI) (CA INDEX NAME)

RN 875656-87-4 HCAPLUS

CN Propanoic acid, 2-[4-[[(2-furanylmethyl)]2-(3-methyl-1-phenyl-1H-pyrazol-4-yl)ethyl]amino]methyl]-2,6-dimethylphenoxy]-2-methyl- (9CI) (CA INDEX NAME)

RN 875656-96-5 HCAPLUS

CN Propanoic acid, 2-[4-[[(2-amino-2-oxoethyl)] ((5-methyl-2-phenyl-2H-1,2,3-triazol-4-yl)methyl]amino]methyl]-2,6-dimethylphenoxy]-2-methyl- (9CI) (CA INDEX NAME)

RN 875656-98-7 HCAPLUS

CN Propanoic acid, 2-[2,6-dimethyl-4-[[[2-(methylamino)-2-oxoethyl][(5-methyl-2-phenyl-2H-1,2,3-triazol-4-yl)methyl]amino]methyl]phenoxy]-2-methyl-(9CI) (CA INDEX NAME)

RN 875657-01-5 HCAPLUS

CN Propanoic acid, 2-[4-[[[2-(dimethylamino)-2-oxoethyl][(5-methyl-2-phenyl-2H-1,2,3-triazol-4-yl)methyl]amino]methyl]-2,6-dimethylphenoxy]-2-methyl-(9CI) (CA INDEX NAME)

RN 875657-02-6 HCAPLUS

CN Propanoic acid, 2-[2,6-dimethyl-4-[[[(5-methyl-1,3,4-oxadiazol-2-yl)methyl][(5-methyl-2-phenyl-2H-1,2,3-triazol-4-yl)methyl]amino]methyl]phenoxy]-2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & Me \\ & HO_2C-C-O \\ & Me \\$$

RN 875657-03-7 HCAPLUS

CN Propanoic acid, 2-[4-[[(3-methoxypropyl)](5-methyl-2-phenyl-2H-1,2,3-triazol-4-yl)methyl]amino]methyl]-2,6-dimethylphenoxy]-2-methyl- (9CI) (CA INDEX NAME)

RN 875657-04-8 HCAPLUS

CN Propanoic acid, 2-[4-[[(2-methoxyethyl)[(5-methyl-2-phenyl-2H-1,2,3-triazol-4-yl)methyl]amino]methyl]-2,6-dimethylphenoxy]-2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{CH}_2-\text{CH}_2-\text{OMe} \\ \\ \text{N} \\ \\ \text{Me} \end{array}$$

$$\begin{array}{c|c} \text{Me} & \text{Me} \\ \hline \\ \text{Ne} & \text{Me} \\ \\ \text{Me} & \text{Me} \\ \\ \text{Me} & \text{Me} \\ \end{array}$$

RN 875657-05-9 HCAPLUS

CN Propanoic acid, 2-[4-[[(2-methoxyethyl)[[5-methyl-2-(4-methylphenyl)-2H-1,2,3-triazol-4-yl]methyl]amino]methyl]-2,6-dimethylphenoxy]-2-methyl-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{CH}_2\text{-CH}_2\text{-OMe} \\ \hline & \text{N} & \text{CH}_2\text{-N-R} \\ \\ & \text{Me} \end{array}$$

RN 875657-06-0 HCAPLUS

CN Propanoic acid, 2-[2,6-dimethyl-4-[[[2-(methylamino)-2-oxoethyl][[5-methyl-2-(4-methylphenyl)-2H-1,2,3-triazol-4-yl]methyl]amino]methyl]phenoxy]-2-methyl- (9CI) (CA INDEX NAME)

RN 875657-07-1 HCAPLUS

CN Propanoic acid, 2-[2,6-dimethyl-4-[[[[5-methyl-2-(4-methylphenyl)-2H-1,2,3-triazol-4-yl]methyl][(5-methyl-1,3,4-oxadiazol-2-yl)methyl]amino]methyl]phenoxy]-2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{HO}_2\text{C}-\text{C}-\text{O} \\ \text{Me} \\$$

RN 875657-08-2 HCAPLUS

CN Propanoic acid, 2-[4-[[(3-methoxypropyl)][[5-methyl-2-(4-methylphenyl)-2H-1,2,3-triazol-4-yl]methyl]amino]methyl]-2,6-dimethylphenoxy]-2-methyl-(9CI) (CA INDEX NAME)

RN 875657-09-3 HCAPLUS

CN Propanoic acid, 2-[4-[[(3-methoxypropyl)[[5-methyl-2-(4-methylphenyl)-2H-1,2,3-triazol-4-yl]methyl]amino]methyl]-2,6-dimethylphenoxy]-2-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

Me Me Me Me Me
$$O-C-CO_2H$$
 Me Me

• HCl

RN 875657-10-6 HCAPLUS

CN Propanoic acid, 2-[4-[[(2-methoxyethyl)[[5-methyl-2-(3-methylphenyl)-2H-1,2,3-triazol-4-yl]methyl]amino]methyl]-2,6-dimethylphenoxy]-2-methyl-

(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{CH}_2-\text{CH}_2-\text{OMe} \\ \hline \\ N & \text{CH}_2-\text{N}-\text{R} \\ \\ \text{Me} & \end{array}$$

RN 875657-11-7 HCAPLUS

CN Propanoic acid, 2-[4-[[(2-methoxyethyl)[[5-methyl-2-(3-methylphenyl)-2H-1,2,3-triazol-4-yl]methyl]amino]methyl]-2,6-dimethylphenoxy]-2-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{CH}_2-\text{CH}_2-\text{OMe} \\ \\ \text{N} \\ \text{Me} \end{array}$$

HCl

RN 875657-12-8 HCAPLUS
CN Propanoic acid, 2-[2,6-dimethyl-4-[[[2-(methylamino)-2-oxoethyl][[5-methyl-2-(3-methylphenyl)-2H-1,2,3-triazol-4-yl]methyl]amino]methyl]phenoxy]-2-methyl- (9CI) (CA INDEX NAME)

RN 875657-13-9 HCAPLUS

CN Propanoic acid, 2-[2,6-dimethyl-4-[[[[5-methyl-2-(3-methylphenyl)-2H-1,2,3-triazol-4-yl]methyl][(5-methyl-1,3,4-oxadiazol-2-yl)methyl]amino]methyl]phenoxy]-2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{HO}_2\text{C}-\text{C}-\text{O} \\ \text{Me} \\$$

RN 875657-14-0 HCAPLUS

CN Propanoic acid, 2-[4-[[(3-methoxypropyl)][[5-methyl-2-(3-methylphenyl)-2H-1,2,3-triazol-4-yl]methyl]amino]methyl]-2,6-dimethylphenoxy]-2-methyl-(9CI) (CA INDEX NAME)

RN 875657-15-1 HCAPLUS

CN Propanoic acid, 2-[4-[[(3-methoxypropyl)[[5-methyl-2-(3-methylphenyl)-2H-1,2,3-triazol-4-yl]methyl]amino]methyl]-2,6-dimethylphenoxy]-2-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 875657-16-2 HCAPLUS

CN Propanoic acid, 2-[4-[[[[2-(4-chlorophenyl)-5-methyl-2H-1,2,3-triazol-4-yl]methyl][2-(methylamino)-2-oxoethyl]amino]methyl]-2,6-dimethylphenoxy]-2-methyl- (9CI) (CA INDEX NAME)

RN 875657-17-3 HCAPLUS

CN Propanoic acid, 2-[4-[[[[2-(4-chlorophenyl)-5-methyl-2H-1,2,3-triazol-4-yl]methyl][(5-methyl-1,3,4-oxadiazol-2-yl)methyl]amino]methyl]-2,6-dimethylphenoxy]-2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{HO}_2\text{C}-\text{C}-\text{O} \\ \text{Me} \\$$

RN 875657-18-4 HCAPLUS

CN Propanoic acid, 2-[4-[[[[2-(3-chlorophenyl)-5-methyl-2H-1,2,3-triazol-4-yl]methyl][2-(methylamino)-2-oxoethyl]amino]methyl]-2,6-dimethylphenoxy]-2-

methyl- (9CI) (CA INDEX NAME)

RN 875657-19-5 HCAPLUS

CN Propanoic acid, 2-[4-[[[[2-(3-chlorophenyl)-5-methyl-2H-1,2,3-triazol-4-yl]methyl][(5-methyl-1,3,4-oxadiazol-2-yl)methyl]amino]methyl]-2,6-dimethylphenoxy]-2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{HO}_2\text{C}-\text{C}-\text{O} \\ \text{Me} \\$$

RN 875657-20-8 HCAPLUS

CN Propanoic acid, 2-[4-[[[[2-(4-methoxyphenyl)-5-methyl-2H-1,2,3-triazol-4-yl]methyl][(5-methyl-1,3,4-oxadiazol-2-yl)methyl]amino]methyl]-2,6-dimethylphenoxy]-2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{HO}_2\text{C}-\text{C}-\text{O} \\ \text{Me} \\ \text{Me} \\ \text{Me} \\ \text{Me} \\ \text{Me} \\ \text{Me} \\ \text{O} \\ \text{Me} \\$$

RN 875657-21-9 HCAPLUS

CN Propanoic acid, 2-[4-[[[2-(4-methoxyphenyl)-5-methyl-2H-1,2,3-triazol-4-yl]methyl][2-(methylamino)-2-oxoethyl]amino]methyl]-2,6-dimethylphenoxy]-2-methyl- (9CI) (CA INDEX NAME)

RN 875657-22-0 HCAPLUS

CN Propanoic acid, 2-[4-[[[[2-(3,4-dimethylphenyl)-5-methyl-2H-1,2,3-triazol-4-yl]methyl][2-(methylamino)-2-oxoethyl]amino]methyl]-2,6-dimethylphenoxy]-2-methyl-(9CI) (CA INDEX NAME)

RN 875657-23-1 HCAPLUS

CN Propanoic acid, 2-[4-[[[[2-[4-(2-methoxyethoxy)phenyl]-5-methyl-2H-1,2,3-triazol-4-yl]methyl][2-(methylamino)-2-oxoethyl]amino]methyl]-2,6-dimethylphenoxy]-2-methyl- (9CI) (CA INDEX NAME)

RN 875657-24-2 HCAPLUS

CN Propanoic acid, 2-[2,6-dimethyl-4-[[[2-(methylamino)-2-oxoethyl][2-(5-methyl-2-phenyl-2H-1,2,3-triazol-4-yl)ethyl]amino]methyl]phenoxy]-2-methyl-(9CI) (CA INDEX NAME)

RN 875657-25-3 HCAPLUS

CN Propanoic acid, 2-[4-[[(2-amino-2-oxoethyl)][2-(5-methyl-2-phenyl-2H-1,2,3-triazol-4-yl)ethyl]amino]methyl]-2,6-dimethylphenoxy]-2-methyl- (9CI) (CA TNDEX NAME)

RN 875657-26-4 HCAPLUS

CN Propanoic acid, 2-[2,6-dimethyl-4-[[[(5-methyl-1,3,4-oxadiazol-2-yl)methyl][2-(5-methyl-2-phenyl-2H-1,2,3-triazol-4-yl)ethyl]amino]methyl]phenoxy]-2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} \\ & \text{HO}_2\text{C}-\text{C}-\text{O} \\ & \text{Me} \end{array}$$

RN 875657-27-5 HCAPLUS

CN Propanoic acid, 2-[4-[[(2-methoxyethyl)[(3-methyl-1-phenyl-1H-pyrazol-4-yl)methyl]amino]methyl]-2,6-dimethylphenoxy]-2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Ph} \\ & & \\ & \text{N} \\ & \text{CH}_2 \\ & \text{N-CH}_2\text{-CH}_2\text{-OMe} \\ & \text{CH}_2 \\ & & \text{CH}_2 \\ & & \text{Me} \\ & & \text{HO}_2\text{C-C-O} \\ & & \text{Me} \end{array}$$

RN 875657-28-6 HCAPLUS

CN Propanoic acid, 2-[2,6-dimethyl-4-[[[(3-methyl-1-phenyl-1H-pyrazol-4-yl)methyl](3,3,3-trifluoropropyl)amino]methyl]phenoxy]-2-methyl- (9CI) (CA INDEX NAME)

RN 875657-29-7 HCAPLUS
CN Propanoic acid, 2-[2,6-dimethyl-4-[[[(3-methyl-1-phenyl-1H-pyrazol-4-yl)methyl](3,3,3-trifluoropropyl)amino]methyl]phenoxy]-2-methyl-, hydrochloride (9CI) (CA INDEX NAME)

RN 875657-30-0 HCAPLUS
CN Propanoic acid, 2-[2,6-dimethyl-4-[[[2-(methylamino)-2-oxoethyl][(3-methyl-1-phenyl-1H-pyrazol-4-yl)methyl]amino]methyl]phenoxy]-2-methyl- (9CI) (CA INDEX NAME)

RN 875657-31-1 HCAPLUS
CN Propanoic acid, 2-[4-[[[2-(dimethylamino)-2-oxoethyl][(3-methyl-1-phenyl-1+-pyrazol-4-yl)methyl]amino]methyl]-2,6-dimethylphenoxy]-2-methyl- (9CI) (CA INDEX NAME)

RN 875657-32-2 HCAPLUS
CN Propanoic acid, 2-[4-[[(5-isoxazolylmethyl)[(3-methyl-1-phenyl-1H-pyrazol-4-yl)methyl]amino]methyl]-2,6-dimethylphenoxy]-2-methyl- (9CI) (CA INDEX NAME)

RN 875657-33-3 HCAPLUS

CN Propanoic acid, 2-[4-[[[1-(4-chlorophenyl)-3-methyl-1H-pyrazol-4-yl]methyl][2-(methylamino)-2-oxoethyl]amino]methyl]-2,6-dimethylphenoxy]-2-methyl- (9CI) (CA INDEX NAME)

PAGE 1-A

Me
$$CH_2$$

N CH_2

N CH_2

CH CH_2

CH CH_2

O

Me Me

RN 875657-34-4 HCAPLUS

CN Propanoic acid, 2-[4-[[[[2-(3,4-dimethylphenyl)-5-methyl-2H-1,2,3-triazol-4-yl]methyl][(5-methyl-1,3,4-oxadiazol-2-yl)methyl]amino]methyl]-2,6-dimethylphenoxy]-2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{HO}_2\text{C}-\text{C}-\text{O} \\ \text{Me} \\$$

RN 875657-35-5 HCAPLUS

CN Propanoic acid, 2-[4-[[[[2-(4-chlorophenyl)-5-methyl-2H-1,2,3-triazol-4-yl]methyl](2-methoxyethyl)amino]methyl]-2,6-dimethylphenoxy]-2-methyl-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{C1} & \text{CH}_2\text{--}\text{CH}_2\text{--}\text{OMe} \\ \hline & \text{N} & \text{CH}_2\text{--}\text{N}\text{---}\text{R} \\ \\ & \text{Me} \end{array}$$

RN 875657-36-6 HCAPLUS

CN Propanoic acid, 2-[4-[[(2-methoxyethyl)[[2-(4-methoxyphenyl)-5-methyl-2H-

1,2,3-triazol-4-yl]methyl]amino]methyl]-2,6-dimethylphenoxy]-2-methyl-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{MeO} & \text{CH}_2\text{--}\text{CH}_2\text{--}\text{OMe} \\ \hline & \text{N} & \text{CH}_2\text{--}\text{N}\text{---}\text{R} \\ \\ & \text{Me} \end{array}$$

RN 875657-37-7 HCAPLUS

CN Propanoic acid, 2-[4-[[(2-hydroxyethyl)[(5-methyl-2-phenyl-2H-1,2,3-triazol-4-yl)methyl]amino]methyl]-2,6-dimethylphenoxy]-2-methyl- (9CI) (CA INDEX NAME)

RN 875657-38-8 HCAPLUS

CN Propanoic acid, 2-[4-[[(2-methoxyethyl)[[1-(4-methylphenyl)-1H-1,2,3-triazol-4-yl]methyl]amino]methyl]-2,6-dimethylphenoxy]-2-methyl- (9CI) (CA INDEX NAME)

$$CH_2-CH_2-OMe$$
 N
 N
 R
 R
 R

RN 875657-39-9 HCAPLUS
CN Propanoic acid, 2-[2,6-dimethyl-4-[[[(5-methyl-1,3,4-oxadiazol-2-yl)methyl][[1-(4-methylphenyl)-1H-1,2,3-triazol-4-yl]methyl]amino]methyl]phenoxy]-2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{HO}_2\text{C}-\text{C}-\text{O} \\ \text{Me} \\ \\ \text$$

RN 875657-40-2 HCAPLUS
CN Propanoic acid, 2-[4-[[(2,2-difluoroethyl)[(5-methyl-2-phenyl-2H-1,2,3-triazol-4-yl)methyl]amino]methyl]-2,6-dimethylphenoxy]-2-methyl- (9CI) (CA INDEX NAME)

875657-41-3 HCAPLUS RN

Propanoic acid, 2-[4-[((2,2-difluoroethyl)]((5-methyl-2-phenyl-2H-1,2,3-CN triazol-4-yl) methyl]amino]methyl]-2,6-dimethylphenoxy]-2-methyl-, hydrochloride (5:3) (9CI) (CA INDEX NAME)

●3/5 HCl

REFERENCE COUNT:

THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 3 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN

19

ACCESSION NUMBER:

2006:75092 HCAPLUS

DOCUMENT NUMBER:

144:170792

TITLE:

Preparation of trisubstituted nitrogen modulators, particularly N, N-dibenzylarylsulfonamide inhibitors, of tyrosine phosphatases for treating metabolic

disorders, autoimmune diseases and neoplasm

INVENTOR(S):

Semple, Joseph E.; Rideout, Darryl; Nutt, Ruth F.; Shernderovich, Mark; Wang, Jing; Mylvaganam, Shankari;

Wu, Feiyue; Tsai, Chung-Ying; Yalamoori, Venkatachalapathi; Loweth, Colin J.

PATENT ASSIGNEE(S):

Cengent Therapeutics, Inc., USA

SOURCE:

PCT Int. Appl., 238 pp.

DOCUMENT TYPE:

CODEN: PIXXD2

Patent

LANGUAGE: FAMILY ACC. NUM. COUNT: English

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
WO 2006009876	A2	20060126	WO 2005-US21540	20050617		
WO 2006009876	A3	20060330				

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,

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CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
            GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ,
             LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA,
             NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK,
             SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU,
             ZA, ZM, ZW
        RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF,
             CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM,
             KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG,
             KZ, MD, RU, TJ, TM
    US 2006135773
                                20060622
                                            US 2005-156230
                                                                    20050617
                          Α1
PRIORITY APPLN. INFO.:
                                            US 2004-581251P
                                                                 Р
                                                                    20040617
                                            US 2004-634200P
                                                                 Ρ
                                                                    20041207
                                            US 2004-638419P
                                                                 P
                                                                    20041222
                         MARPAT 144:170792
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OTHER SOURCE(S): MAR

$$G^2-L^2$$
 $N-L^3$
 G^1-L^1

AB The invention is related to the preparation of trisubstituted nitrogen compds. I [L1-L3 = independently N-C single bond (G1, G2, or G3 are directly bonded to N by a single bond), alkylene, sulfonyl, amido, etc.; G1-G3 = alkyl, aryl, cyanobiaryl, etc., optionally substituted with carboxy, phosphonato, phosphonatoalkyl, phosphonatohaloalkyl, amido, etc.], and their pharmaceutically acceptable derivs., including N,Ndibenzylarylsulfonamides. The invention is also related to the use of compds. I, and their compns., for modulating the activity of protein tyrosine phosphatases, especially PTP-1B. Thus, reacting (bromodifluoromethyl) phosphonic acid di-Et ester with bis(4iodobenzyl)carbamic acid tert-Bu ester (preparation given), followed by reaction with 2-chlorobenzenesulfonyl chloride and ester hydrolysis gave phosphonic acid II. In a pNPP assay, selected I displayed IC50 values of less than 99 nM for the inhibition of PTP-1B. I are useful for treating metabolic disorders, autoimmune diseases and neoplasm.

IT 874567-71-2P, 2-Carboxymethoxy-5-[[(4-methylsulfonylbenzyl)(2-methoxyphenylsulfonyl)amino]methyl]benzoic acid 874568-56-6P,
5-[[[(Biphenyl-2-yl)methyl](2-methoxyphenylsulfonyl)amino]methyl]-2(carboxymethoxy)benzoic acid
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of N,N-dibenzylarylsulfonamide inhibitors of tyrosine phosphatases for treating metabolic disorders, autoimmune diseases and neoplasm)

RN 874567-71-2 HCAPLUS

CN Benzoic acid, 2-(carboxymethoxy)-5-[[[(2-methoxyphenyl)sulfonyl][[4-(methylsulfonyl)phenyl]methyl]amino]methyl]- (9CI) (CA INDEX NAME)

$$O = S - Me$$

$$O = S - Me$$

$$CO_2H$$

$$CH_2 O$$

$$CH_2 O$$

$$CH_2 - N - S$$

$$CH_2 - N - S$$

RN 874568-56-6 HCAPLUS

CN Benzoic acid, 5-[[([1,1'-biphenyl]-2-ylmethyl)[(2-methoxyphenyl)sulfonyl]amino]methyl]-2-(carboxymethoxy)- (9CI) (CA INDEX NAME)

$$HO_2C$$
 Ph CH_2 O OMe CH_2 O OMe OMe

L4 ANSWER 4 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:1103761 HCAPLUS

DOCUMENT NUMBER: 143:387018

TITLE: Preparation of oxazole compounds containing

phenoxyacetic acid moiety as PPAR α/γ

agonists

INVENTOR(S): Kagechika, Hiroyuki; Shibata, Yoshihiro; Oguri,

Atsushi

PATENT ASSIGNEE(S): Daiichi Pharmaceutical Co. Ltd., Japan

SOURCE:

PCT Int. Appl., 171 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.						KIND DATE			1	APPL:	ICAT	ION		DATE						
		2005		_		A1 20051013 C1 20060105			,	WO 2	005-	JP57	20050328							
	,,,	W:	AE, CN, GE, LK, NO, SY, BW, AZ, EE, RO,	AG, CO, GH, LR, NZ, TJ, GH, BY, ES, SE,	AL, CR, GM, LS, OM, TM, GM, KG,	AM, CU, HR, LT, PG, TN, KE, KZ, FR, SK,	AT, CZ, HU, LU, PH, TR, LS, MD, GB, TR,	AU, DE, ID, LV, PL, TT, MW, RU, GR,	AZ, DK, IL, MA, PT, TZ, MZ, TJ,	DM, IN, MD, RO, UA, NA, TM, IE,	DZ, IS, MG, RU, UG, SD, AT, IS,	EC, JP, MK, SC, US, SL, BE, IT,	EE, KE, MN, SD, UZ, SZ, BG, LT,	EG, KG, MW, SE, VC, TZ, CH, LU,	ES, KP, MX, SG, VN, UG, CY, MC,	BZ, FI, KR, MZ, SK, YU, ZM, CZ, NL, GQ,	GB, KZ, NA, SL, ZA, ZW, DE, PL,	GD, LC, NI, SM, ZM, AM, DK, PT,	ZW	
	PRIORITY APPLN. INFO.:						MADDAT 1/2.207010					JP 2004-99201 JP 2005-15954					A 20040330 A 20050124			

OTHER SOURCE(S):

MARPAT 143:387018

GI

AB Title compds. I [Q = optionally substituted benzene, pyridine with OH, halo, alkenyl, etc.; R1 = optionally substituted Ph, pyridyl, pyrimidinyl, etc. with halo, alkenyl, alkoxy, etc.; R2 = optionally substituted pyridyl, pyrimidinyl, pyrazinyl, etc. with OH, halo, alkenyl, etc.; X, Y, Z = C, O, S, etc.; R3-R6 = H, alkyl, etc.; R7-R9 = H, alkyl; n = 0-3] were prepared For example, reductive amination of 2-formylthiazole with compound

II

```
II [R = H; OR' = tert-butoxy], e.g., prepared from 2-(3-bromophenyl)-4-
     chloromethyl-5-methylphenyloxazole in 4 steps, followed by treatment with
     HCl afforded compound II [R = thiazol-2-ylmethyl; OR' = OH] hydrochloride
            In GAL4-hPPAR transactivation assays, compound II [R =
     thiazol-2-ylmethyl; OR' = OH] hydrochloride salt showed the EC50 value of
     0.013 \muM for PPAR\alpha. Of note, compds. I are useful as PPAR
     \alpha/\gamma agonists for the treatment of diabetes.
ΙT
     866639-69-2P 866639-72-7P 866639-76-1P
     866639-78-3P 866639-80-7P 866639-82-9P
     866639-84-1P 866639-86-3P 866639-88-5P
     866639-92-1P 866639-94-3P 866639-96-5P
     866639-98-7P 866640-00-8P 866640-02-0P
     866640-04-2P 866640-06-4P 866640-10-0P
     866640-12-2P 866640-14-4P 866640-16-6P
     866640-18-8P 866640-20-2P 866640-22-4P
     866640-24-6P 866640-26-8P 866640-28-0P
     866640-30-4P 866640-32-6P 866640-34-8P
     866640-36-0P 866640-38-2P 866640-42-8P
     866640-44-0P 866640-46-2P 866640-48-4P
     866640-50-8P 866640-53-1P 866640-59-7P
     866640-62-2P 866640-64-4P 866640-66-6P
     866640-68-8P 866640-69-9P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
        (preparation of oxazole compds. containing phenoxyacetic acid moiety as PPAR
        \alpha/\gamma agonists)
RN
     866639-69-2 HCAPLUS
CN
     Propanoic acid, 2-methyl-2-[4-[[[2-(methylamino)-2-oxoethyl][(5-methyl-2-
     phenyl-4-oxazolyl) methyl] amino] methyl] -2-(2-propenyl) phenoxy] -,
     trifluoroacetate (9CI) (CA INDEX NAME)
     CM
          1
          866639-68-1
     CRN
     CMF
         C28 H33 N3 O5
                                   Me
                 H_2C = CH - CH_2
                                   C-CO2H
        MeNH-C
                                   Me
            CH<sub>2</sub>
                N-CH2
         Me
     CM
          2
```

CRN

CMF

76-05-1

C2 H F3 O2

RN 866639-72-7 HCAPLUS

CN Propanoic acid, 2-[4-[[[[2-(3-bromophenyl)-5-methyl-4-oxazolyl]methyl][2-(methylamino)-2-oxoethyl]amino]methyl]-2-(2-propenyl)phenoxy]-2-methyl-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 866639-71-6 CMF C28 H32 Br N3 O5

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 866639-76-1 HCAPLUS

CN Propanoic acid, 2-[2,6-dimethyl-4-[[[(5-methyl-2-phenyl-4-oxazolyl)methyl](2-oxazolylmethyl)amino]methyl]phenoxy]-2-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} \\ & \text{HO}_2\text{C}-\text{C}-\text{O} \\ & \text{Me} \\ & \text{Ph} \\ & \text{Me} \\ &$$

● HCl

RN 866639-78-3 HCAPLUS

CN Propanoic acid, 2-[2,6-dimethyl-4-[[[2-(methylamino)-2-oxoethyl]](5-methyl-2-phenyl-4-oxazolyl)methyl]amino]methyl]phenoxy]-2-methyl- (9CI) (CA INDEX NAME)

RN 866639-80-7 HCAPLUS

CN Propanoic acid, 2-[4-[[[2-(dimethylamino)-2-oxoethyl][(5-methyl-2-phenyl-4-oxazolyl)methyl]amino]methyl]-2,6-dimethylphenoxy]-2-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 866639-82-9 HCAPLUS
CN Propanoic acid, 2-[2,6-dimethyl-4-[[[(5-methyl-2-phenyl-4-oxazolyl)methyl](2-thiazolylmethyl)amino]methyl]phenoxy]-2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} \\ & \text{HO}_2\text{C}-\text{C}-\text{O} \\ & \text{Me} \end{array}$$

RN 866639-84-1 HCAPLUS
CN Propanoic acid, 2-[4-[[[(4,5-dihydro-5-oxo-1,3,4-oxadiazol-2-yl)methyl][(5-methyl-2-phenyl-4-oxazolyl)methyl]amino]methyl]-2,6-dimethylphenoxy]-2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{HO}_2\text{C}-\text{C}-\text{O} \\ \text{Me} \\ \text{Me} \\ \text{Me} \\ \text{Me} \\ \text{Me} \\ \text{Me} \\ \text{O} \\ \text{O} \\ \text{Me} \\ \text{O} \\ \text{Me} \\ \text{$$

RN 866639-86-3 HCAPLUS

CN Propanoic acid, 2-[2,6-dimethyl-4-[[[(5-methyl-1,3,4-oxadiazol-2-yl)methyl][(5-methyl-2-phenyl-4-oxazolyl)methyl]amino]methyl]phenoxy]-2-methyl-, hydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{HO}_2\text{C}-\text{C}-\text{O} \\ \text{Me} \end{array}$$

•x HCl

RN 866639-88-5 HCAPLUS

CN Propanoic acid, 2-[2,6-dimethyl-4-[[[(3-methyl-1,2,4-oxadiazol-5-yl)methyl][(5-methyl-2-phenyl-4-oxazolyl)methyl]amino]methyl]phenoxy]-2-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} \\ & \text{HO}_2\text{C}-\text{C}-\text{O} \\ & \text{Me} \end{array}$$

● HCl

RN 866639-92-1 HCAPLUS
CN Propanoic acid, 2-[2,6-dimethyl-4-[[[2-(5-methyl-2-phenyl-4-oxazolyl)ethyl](2-thiazolylmethyl)amino]methyl]phenoxy]-2-methyl-, dihydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{HO}_2\text{C}-\text{C}-\text{O} \\ \text{Me} \\ \text{Me} \\ \text{Me} \\ \text{Me} \\ \text{Me} \\ \text{CH}_2 \\ \text{CH}_2 - \text{CH}_2 - \text{CH}_2 - \text{CH}_2 \\ \text{O} \\ \text{Me} \\ \end{array}$$

●2 HC1

RN 866639-94-3 HCAPLUS
CN Propanoic acid, 2-[4-[[(2-benzoxazolylmethyl)[(5-methyl-2-phenyl-4-oxazolyl)methyl]amino]methyl]-2,6-dimethylphenoxy]-2-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

HCl

$$\begin{array}{c} \text{Me} \\ \text{HO}_2\text{C}-\text{C}-\text{O} \\ \text{Me} \\$$

● HCl

RN 866639-98-7 HCAPLUS
CN Propanoic acid, 2-[2,6-dimethyl-4-[[[(4-methyl-2-oxazolyl)methyl][(5-methyl-2-phenyl-4-oxazolyl)methyl]amino]methyl]phenoxy]-2-methyl-,
monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{HO}_2\text{C}-\text{C}-\text{O} \\ \text{Me} \\$$

● HCl

RN 866640-00-8 HCAPLUS
CN Propanoic acid, 2-[2,6-dimethyl-4-[[(2-oxazolylmethyl)[(5-phenyl-1,3,4-oxadiazol-2-yl)methyl]amino]methyl]phenoxy]-2-methyl-, hydrochloride (4:1) (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{HO}_2\text{C}-\text{C}-\text{O} \\ \text{Me} \\$$

●1/4 HCl

RN 866640-02-0 HCAPLUS
CN Propanoic acid, 2-[2,6-dimethyl-4-[[(2-oxazolylmethyl)[(5-phenyl-2-oxazolyl)methyl]amino]methyl]phenoxy]-2-methyl-, hydrochloride (4:3) (9CI) (CA INDEX NAME)

CN

$$\begin{array}{c|c} & \text{Me} \\ & \text{HO}_2\text{C}-\text{C}-\text{O} \\ & \text{Me} \\ &$$

●3/4 HCl

RN 866640-04-2 HCAPLUS

Propanoic acid, 2-[2,6-dimethyl-4-[[(2-oxazolylmethyl)[[5-(2-thienyl)-1,3,4-oxadiazol-2-yl]methyl]amino]methyl]phenoxy]-2-methyl-, hydrochloride (2:1) (9CI) (CA INDEX NAME)

RN 866640-06-4 HCAPLUS

CN Propanoic acid, 2-[2,6-dimethyl-4-[[(2-oxazolylmethyl)[[3-(2-thienyl)-1,2,4-oxadiazol-5-yl]methyl]amino]methyl]phenoxy]-2-methyl- (9CI) (CA INDEX NAME)

RN 866640-10-0 HCAPLUS

CN Propanoic acid, 2-[2-methoxy-6-methyl-4-[[[(5-methyl-2-phenyl-4-oxazolyl)methyl](2-oxazolylmethyl)amino]methyl]phenoxy]-2-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} \\ & \text{HO}_2\text{C}-\text{C}-\text{O} \\ & \text{Me} \\ &$$

● HCl

RN 866640-12-2 HCAPLUS

CN Propanoic acid, 2-[2,6-dimethyl-4-[[[[5-methyl-2-(4-methylphenyl)-4-oxazolyl]methyl][(5-methyl-1,3,4-oxadiazol-2-yl)methyl]amino]methyl]phenoxy]-2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{HO}_2\text{C}-\text{C}-\text{O} \\ \text{Me} \\$$

RN 866640-14-4 HCAPLUS
CN Propanoic acid, 2-[4-[[[[2-(4-chlorophenyl)-5-methyl-4-oxazolyl]methyl][(5-methyl-1,3,4-oxadiazol-2-yl)methyl]amino]methyl]-2,6-dimethylphenoxy]-2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} \\ & \text{HO}_2\text{C}-\text{C}-\text{O} \\ & \text{Me} \end{array}$$

RN 866640-16-6 HCAPLUS
CN Propanoic acid, 2-[2,6-dimethyl-4-[[[(3-phenyl-1,2,4-oxadiazol-5-yl)methyl](2-thiazolylmethyl)amino]methyl]phenoxy]-2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} \\ & \text{HO}_2\text{C}-\text{C}-\text{O} \\ & \text{Me} \\ &$$

RN 866640-18-8 HCAPLUS
CN Propanoic acid, 2-[2,6-dimethyl-4-[[[(5-phenyl-2-oxazolyl)methyl](2-thiazolylmethyl)amino]methyl]phenoxy]-2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{HO}_2\text{C}-\text{C}-\text{O} \\ \text{Me} \\ \text{Me} \\ \text{Me} \\ \text{Me} \\ \text{Me} \\ \text{CH}_2 \\ \text{N} \\ \text{CH}_2 \\ \text{N} \\ \text{O} \\ \end{array}$$

RN 866640-20-2 HCAPLUS

CN Propanoic acid, 2-[2,6-dimethyl-4-[[[[5-methyl-2-(5-methyl-2-thienyl)-4-oxazolyl]methyl](2-thiazolylmethyl)amino]methyl]phenoxy]-2-methyl- (9CI) (CA INDEX NAME)

RN 866640-22-4 HCAPLUS

CN Propanoic acid, 2-[2,6-dimethyl-4-[[[[5-methyl-2-(5-methyl-2-thienyl)-4-oxazolyl]methyl](2-oxazolylmethyl)amino]methyl]phenoxy]-2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{Me} \\ \text{Me} \\ \text{Me} \\ \text{Me} \\ \text{Me} \\ \text{CH}_2 - \text{N-CH}_2 \\ \text{Me} \\ \text{Me} \\ \text{Me} \\ \end{array}$$

RN 866640-24-6 HCAPLUS

CN Propanoic acid, 2-[2,6-dimethyl-4-[[[[5-methyl-2-(5-methyl-2-thienyl)-4-oxazolyl]methyl][(5-methyl-2-oxazolyl)methyl]amino]methyl]phenoxy]-2-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} \\ & \text{HO}_2\text{C}-\text{C}-\text{O} \\ & \text{Me} \\ &$$

● HCl

RN 866640-26-8 HCAPLUS

CN Propanoic acid, 2-[2,6-dimethyl-4-[[[(5-methyl-2-oxazolyl)methyl][(3-phenyl-1,2,4-oxadiazol-5-yl)methyl]amino]methyl]phenoxy]-2-methyl-, hydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{HO}_2\text{C}-\text{C}-\text{O} \\ \text{Me} \\ \text{Me} \\ \text{Me} \\ \text{Me} \\ \text{Me} \\ \text{Me} \\ \text{O} \\ \text{CH}_2 \\ \text{N} \\ \text{O} \\ \text{N} \end{array} \qquad \begin{array}{c} \text{Me} \\ \text{Me} \\ \text{O} \\ \text{N} \\ \text{O} \\ \text{N} \end{array}$$

•x HCl

RN 866640-28-0 HCAPLUS
CN Propanoic acid, 2-[2,6-dimethyl-4-[[[(5-methyl-2-oxazolyl)methyl][(5-phenyl-2-oxazolyl)methyl]amino]methyl]phenoxy]-2-methyl-, hydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{HO}_2\text{C}-\text{C}-\text{O} \\ \text{Me} \\ \text{Me} \\ \text{Me} \\ \text{Me} \\ \text{Me} \\ \text{Me} \\ \text{Ph} \\ \text{Ph} \\ \end{array}$$

●x HCl

RN 866640-30-4 HCAPLUS
CN Propanoic acid, 2-[2,6-dimethyl-4-[[[2-(methylamino)-2-oxoethyl][[5-methyl-2-(4-methylphenyl)-4-oxazolyl]methyl]amino]methyl]phenoxy]-2-methyl- (9CI) (CA INDEX NAME)

RN 866640-32-6 HCAPLUS

CN Propanoic acid, 2-[4-[[[[2-(4-chlorophenyl)-5-methyl-4-oxazolyl]methyl][2-(methylamino)-2-oxoethyl]amino]methyl]-2,6-dimethylphenoxy]-2-methyl-(9CI) (CA INDEX NAME)

RN 866640-34-8 HCAPLUS

CN Propanoic acid, 2-[4-[[[[2-(3-chlorophenyl)-5-methyl-4-oxazolyl]methyl][2-(methylamino)-2-oxoethyl]amino]methyl]-2,6-dimethylphenoxy]-2-methyl-(9CI) (CA INDEX NAME)

RN 866640-36-0 HCAPLUS

CN Propanoic acid, 2-[2-methoxy-6-methyl-4-[[[2-(methylamino)-2-oxoethyl]][(5-methyl-2-phenyl-4-oxazolyl)methyl]amino]methyl]phenoxy]-2-methyl- (9CI) (CA INDEX NAME)

RN 866640-38-2 HCAPLUS

CN Propanoic acid, 2-[2-methoxy-6-methyl-4-[[[(5-methyl-2-phenyl-4-oxazolyl)methyl](2-thiazolylmethyl)amino]methyl]phenoxy]-2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} \\ & \text{HO}_2\text{C}-\text{C}-\text{O} \\ & \text{Me} \\ &$$

RN 866640-42-8 HCAPLUS
CN Propanoic acid, 2-[2,6-dimethyl-4-[[[2-(5-methyl-2-phenyl-4-oxazolyl)ethyl](2-oxazolylmethyl)amino]methyl]phenoxy]-2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{HO}_2\text{C}-\text{C}-\text{O} \\ \text{Me} \\ \text{O} \\ \text{CH}_2-\text{N}-\text{CH}_2-\text{CH}_2-\text{CH}_2 \\ \text{Me} \\ \text$$

RN 866640-44-0 HCAPLUS
CN Propanoic acid, 2-[2,6-dimethyl-4-[[(2-oxazolylmethyl)[(5-phenyl-3-isoxazolyl)methyl]amino]methyl]phenoxy]-2-methyl- (9CI) (CA INDEX NAME)

RN 866640-46-2 HCAPLUS

CN Propanoic acid, 2-[2-ethyl-4-[[[(5-methyl-2-phenyl-4-oxazolyl)methyl](2-oxazolylmethyl)amino]methyl]phenoxy]-2-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} \\ & \text{HO}_2\text{C}-\text{C}-\text{O} \\ & \text{Me} \\ & \text{Et} \\ & \text{CH}_2 \\ & \text{CH}_2-\text{N}-\text{CH}_2 \\ & \text{O} \\ & \text{Me} \\ \end{array}$$

● HCl

RN 866640-48-4 HCAPLUS

CN Propanoic acid, 2-[2-ethyl-6-methyl-4-[[[(5-methyl-2-phenyl-4-oxazolyl)methyl](2-oxazolylmethyl)amino]methyl]phenoxy]-2-methyl-, hydrochloride (20:17) (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} \\ & \text{HO}_2\text{C}-\text{C}-\text{O} \\ & \text{Me} \end{array}$$

●17/20 HCl

RN 866640-50-8 HCAPLUS
CN Propanoic acid, 2-[2,6-dimethyl-4-[[[(5-methyl-2-phenyl-4-oxazolyl)methyl][[5-(trifluoromethyl)-1,3,4-oxadiazol-2-yl]methyl]amino]methyl]phenoxy]-2-methyl-, hydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{HO}_2\text{C}-\text{C}-\text{O} \\ \text{Me} \\$$

•x HCl

RN 866640-53-1 HCAPLUS
CN Propanoic acid, 2-[4-[[[(4,5-dihydro-4-methyl-5-oxo-1,3,4-oxadiazol-2-yl)methyl][(5-methyl-2-phenyl-4-oxazolyl)methyl]amino]methyl]-2,6-dimethylphenoxy]-2-methyl- (9CI) (CA INDEX NAME)

RN 866640-59-7 HCAPLUS

CN Propanoic acid, 2-[2,6-dimethyl-4-[[[[5-methyl-2-(4-methylphenyl)-4-oxazolyl]methyl][(3-methyl-1,2,4-oxadiazol-5-yl)methyl]amino]methyl]phenoxy]-2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} \\ & \text{HO}_2\text{C}-\text{C}-\text{O} \\ & \text{Me} \\ &$$

RN 866640-62-2 HCAPLUS

CN Propanoic acid, 2-[4-[[[2-(cyclopropylamino)-2-oxoethyl]][(5-methyl-2-phenyl-4-oxazolyl)methyl]amino]methyl]-2,6-dimethylphenoxy]-2-methyl-(9CI) (CA INDEX NAME)

RN 866640-64-4 HCAPLUS

CN Propanoic acid, 2-[4-[[[2-[(cyclopropylmethyl)amino]-2-oxoethyl][(5-methyl-2-phenyl-4-oxazolyl)methyl]amino]methyl]-2,6-dimethylphenoxy]-2-methyl-(9CI) (CA INDEX NAME)

RN 866640-66-6 HCAPLUS

CN Propanoic acid, 2-[4-[[[2-(butylamino)-2-oxoethyl][(5-methyl-2-phenyl-4-oxazolyl)methyl]amino]methyl]-2,6-dimethylphenoxy]-2-methyl- (9CI) (CA INDEX NAME)

RN 866640-68-8 HCAPLUS

CN Propanoic acid, 2-[2,6-dimethyl-4-[[[(5-methyl-2-phenyl-4-oxazolyl)methyl][[5-(3-pyridinyl)-1,3,4-oxadiazol-2-yl]methyl]amino]methyl]phenoxy]-2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{HO}_2\text{C}-\text{C}-\text{O} \\ \text{Me} \\$$

RN 866640-69-9 HCAPLUS

CN Propanoic acid, 2-[4-[[(2-amino-2-oxoethyl)](5-methyl-2-phenyl-4-oxazolyl)methyl]amino]methyl]-2,6-dimethylphenoxy]-2-methyl- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN

8

ACCESSION NUMBER:

2005:980891 HCAPLUS

DOCUMENT NUMBER:

143:379070

TITLE:

Minor structural modifications convert a selective

 $PPAR\alpha$ agonist into a potent, highly selective

PPARδ agonist

AUTHOR (S):

Weigand, Stefan; Bischoff, Hilmar;

Dittrich-Wengenroth, Elke; Heckroth, Heike; Lang,

Dieter; Vaupel, Andrea; Woltering, Michael

CORPORATE SOURCE:

Pharma Research, BAYER Health Care AG, Wuppertal,

D-42096, Germany

SOURCE:

Bioorganic & Medicinal Chemistry Letters (2005),

15(20), 4619-4623

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER:

Elsevier B.V.

DOCUMENT TYPE:

Journal English

LANGUAGE: OTHER SOURCE(S):

CASREACT 143:379070

GI

Ι

AB We report the solid-phase synthesis and pharmacol. evaluation of a new series of small-mol. agonists of the human peroxisome proliferator-activated receptor δ (PPAR δ) based on a lead structure from our PPAR α program. Compound I showed good pharmacokinetics.

IT 518336-75-9P 518336-88-4P 866820-82-8P
RL: CPN (Combinatorial preparation); PAC (Pharmacological activity); THU
 (Therapeutic use); BIOL (Biological study); CMBI (Combinatorial study);
 PREP (Preparation); USES (Uses)

(solid-phase preparation of small-mol. PPAR δ agonists and evaluation for possible use for metabolic disorder treatment)

RN 518336-75-9 HCAPLUS

CN Propanoic acid, 2-[4-[[(cyclopropylmethyl)[2-[(2,4-dichlorophenyl)amino]-2-oxoethyl]amino]methyl]-2-methylphenoxy]-2-methyl- (9CI) (CA INDEX NAME)

RN 518336-88-4 HCAPLUS

CN Propanoic acid, 2-[4-[[(cyclohexylmethyl) [2-[(2,4-dichlorophenyl)amino]-2-oxoethyl]amino]methyl]-2-methylphenoxy]-2-methyl- (9CI) (CA INDEX NAME)

RN 866820-82-8 HCAPLUS

Propanoic acid, 2-[4-[[[2-[(2,4-dichlorophenyl)amino]-2-CN oxoethyl]phenylamino]methyl]-2-methylphenoxy]-2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Ph} & \text{O} \\ & \text{HO}_2\text{C} - \text{C} - \text{O} \\ & \text{Me} \end{array} \quad \begin{array}{c|c} \text{Ph} & \text{O} \\ & \text{C} \text{H}_2 - \text{C} - \text{NH} \end{array}$$

REFERENCE COUNT:

13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

HCAPLUS COPYRIGHT 2006 ACS on STN L4 ANSWER 6 OF 26

ACCESSION NUMBER: 2005:921438 HCAPLUS

DOCUMENT NUMBER: 143:259498

TITLE: Discovery and structure-activity relationships of

novel sulfonamides as potent PTP1B inhibitors

AUTHOR (S): Holmes, Christopher P.; Li, Xianfeng; Pan, Yijun; Xu,

Caiding; Bhandari, Ashok; Moody, Claire M.; Miguel, Joy A.; Ferla, Steven W.; De Francisco, M. Nuria; Frederick, Brian T.; Zhou, Siqun; Macher, Natalie; Jang, Larry; Irvine, Jennifer D.; Grove, J. Russell

CORPORATE SOURCE: Affymax, Inc., Palo Alto, CA, 94304, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2005),

15(19), 4336-4341

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 143:259498

A series of novel sulfonamides containing a single difluoromethylenephosphonate group were discovered to be potent inhibitors of protein tyrosine phosphatase 1B. Structure-activity relationships around the scaffold were investigated, leading to the identification of compds. with IC50 or Ki values in the low nanomolar range. These sulfonamide-based inhibitors exhibit 100 and 30 times higher inhibitory activity than the corresponding tertiary amines and carboxamides, resp.

IT 863976-92-5P 863976-94-7P 863976-95-8P RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(discovery and structure-activity relationships of novel sulfonamides as potent PTP1B inhibitors)

RN 863976-92-5 HCAPLUS

CN Acetic acid, [4-[[[[4-(difluorophosphonomethyl)phenyl]methyl](phenylmethyl)amino]sulfonyl]-2-(trifluoromethyl)phenoxy]- (9CI) (CA INDEX NAME)

$$CF_3$$
 CF_2
 CF_2
 CF_2
 CF_2
 CF_2
 CF_2
 CF_2
 CF_2
 CF_2

RN 863976-94-7 HCAPLUS

CN Acetic acid, [4-[[[[4-(difluorophosphonomethyl)phenyl]methyl](phenylmethyl)amino]sulfonyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & & \text{O} & \text{CH}_2-\text{Ph} \\ & & \text{O} & \text{CH}_2-\text{Ph} \\ & & \text{S}-\text{N}-\text{CH}_2 \end{array}$$

RN 863976-95-8 HCAPLUS

CN Acetic acid, [4-[[[[4-(difluorophosphonomethyl)phenyl]methyl] (phenylmethyl)amino]sulfonyl]-2,6-dimethylphenoxy]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & & \text{Me} \\ \text{HO}_2\text{C}-\text{CH}_2-\text{O} & & \text{CH}_2-\text{Ph} \\ & & \text{S}-\text{N}-\text{CH}_2 \\ & & \text{O} \end{array}$$

REFERENCE COUNT:

THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:

2005:638735 HCAPLUS

DOCUMENT NUMBER:

143:153383

TITLE:

Preparation of triazole, oxadiazole and thiadiazole derivatives as PPAR modulators for the treatment of

diabetes

INVENTOR(S):

Mantlo, Nathan Bryan; Navarro, Antonio; Saeed, Ashraf; Gernert, Douglas Linn; Ma, Tianwei; Pfeifer, Lance

Allen

PATENT ASSIGNEE(S):

Eli Lilly and Company, USA

SOURCE:

PCT Int. Appl., 175 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.					KIND DATE					APPL	ICAT:	ION I	DATE					
WO 2005065683					A1	-	20050721		1	WO 2	004-1	US39'	20041221					
	W:	ΑE,	AG,	AL,	AM,	AT,	ΑU,	ΑZ,	BA,	BB,	BG,	BR,	BW,	BY,	ΒZ,	CA,	CH,	
		CN,	CO,	CR,	CU,	CZ,	DΕ,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FΙ,	GB,	GD,	
		GE,	GH,	GM,	HR,	HU,	ID,	ΙL,	IN,	IS,	JP,	ΚE,	KG,	ΚP,	KR,	ΚZ,	LC,	
		LK,	LR,	LS,	LT,	LU,	LV,	ΜA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NI,	
		NO,	ΝZ,	OM,	PG,	PH,	PL,	PΤ,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,	
		ΤJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UΖ,	VC,	VN,	ΥU,	ZA,	ZM,	ZW	
	RW:	BW,	GH,	GM,	KΕ,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	
		ΑZ,	BY,	KG,	ΚZ,	MD,	RU,	ТJ,	TM,	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	
		EE,	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,	IS,	IT,	LT,	LU,	MC,	NL,	PL,	PT,	
		RO,	SE,	SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	
		MR,	ΝE,	SN,	TD,	TG												
AU 2004311909					A1	A1 20050721 AU 2004							311909 200412					
PRIORITY APPLN. INFO.:									1	US 2	003-	5323:	P 20031222					
									US 2004-586563P					P 20040709				
										EP 2	004-3	3801	58	1	A 2	0040	721	
							EP 2	004-3	3801	59	1	A 2	0040	721				
						1	WO 2	004-1	US39	775	Ī	<i>v</i> 2	0041	221				
OTHER SOURCE(S):					MAR	PAT	143:	15338	83									

GI

$$E-Y \xrightarrow{R8} X \xrightarrow{R32} X \xrightarrow{R1} V \xrightarrow{R10} R10$$

$$\begin{array}{c|c} \text{Me} & \text{CF}_3 \\ \text{HO}_2\text{C} & \text{Me} \\ \text{Me} & \text{N} & \text{N} \\ \text{Et} \end{array}$$

II

AΒ The title compds. I [X = a single bond, O, S, SO2 and N; U = an aliphatic] linker; Y = O, C, S, NH and a single bond; W = N, O or S; E = CR3R4A or A (wherein A = carboxy, tetrazole, alkylnitrile, carboxamide, sulfonamide and acylsufonamide; R3 = H, alkyl, alkoxy; R4 = H, alkyl, alkoxy, etc.; or R3 and R4 are optionally combined to form cycloalkyl); V = (hetero)alkyl, a bond; R1 = H, alkyl, heteroaryl, etc.; R8 = H, alkyl, alkenyl, halo; R9 = H, alkyl, halo, etc.; R10, R11 = H, OH, CN, etc.; R32 = a bond, H, halo, alkyl, etc.] which are modulators of peroxisome proliferator activated receptors (PPARs) and are useful for the treatment of diabetes and other metabolic disorders, were prepared and formulated. E.g., a multi-step synthesis of II, starting from Me glycolate and benzyl bromide, was given. The binding and cotransfection efficacy values for compds. I which are especially useful for modulating a PPAR receptor, are ≤ 100 nM and ≥ 50%, resp.

IT 860261-57-0P 860261-58-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of triazole, oxadiazole and thiadiazole derivs. as PPAR modulators for the treatment of diabetes)

RN 860261-57-0 HCAPLUS

CN Propanoic acid, 2-methyl-2-[2-methyl-4-[[methyl[[1-methyl-3-[4-(trifluoromethyl)phenyl]-1H-1,2,4-triazol-5-yl]methyl]amino]methyl]phenoxy
[- (9CI) (CA INDEX NAME)

F₃C
$$\stackrel{\text{Me}}{\underset{\text{N-N}}{\bigvee}}$$
 $\stackrel{\text{Me}}{\underset{\text{CH}_2-\text{N-CH}_2}{\bigvee}}$ $\stackrel{\text{Me}}{\underset{\text{Me}}{\bigvee}}$ $\stackrel{\text{Me}}{\underset{\text{Me}}{\bigvee}}$

RN 860261-58-1 HCAPLUS

CN Propanoic acid, 2-[4-[[[[1-ethyl-3-[4-(trifluoromethyl)phenyl]-1H-1,2,4-triazol-5-yl]methyl]methylamino]methyl]-2-methylphenoxy]-2-methyl- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:479502 HCAPLUS

DOCUMENT NUMBER: 143:172789

TITLE: Design and Synthesis of α -Aryloxyphenylacetic

Acid Derivatives: A Novel Class of PPAR α/γ

Dual Agonists with Potent Antihyperglycemic and Lipid

Modulating Activity

AUTHOR(S): Shi, Guo Q.; Dropinski, James F.; McKeever, Brian M.;

Xu, Shihua; Becker, Joseph W.; Berger, Joel P.;
MacNaul, Karen L.; Elbrecht, Alex; Zhou, Gaochao;
Doebber, Thomas W.; Wang, Peiran; Chao, Yu-Sheng;
Forrest, Mike; Heck, James V.; Moller, David E.;

Jones, A. Brian

CORPORATE SOURCE: Departments of Medicinal Chemistry, Metabolic

Disorders, Atherosclerosis and Endocrinology and Animal Pharmacology, Merck Research Laboratories,

Rahway, NJ, 07065-0900, USA

SOURCE: Journal of Medicinal Chemistry (2005), 48(13),

4457-4468

CODEN: JMCMAR; ISSN: 0022-2623

American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 143:172789

GI

PUBLISHER:

AB The synthesis and structure-activity relationships of novel series of α -aryloxyphenylacetic acids as PPAR α/γ dual agonists are reported. The initial search for surrogates of the ester group in the screen lead led first to the optimization of a subseries I (R1 = Et, Me2CH, Me3C, Ph; R2, R3 = H, Me, Cl, n-Pr, EtCHMe; R4 = H, F3C, Et, Me2CH, Me2CHO, Me2CHCH2) with a ketone moiety. Further efforts to modify the ketone subseries led to the design and synthesis of two new subseries containing fused heterocyclic ring systems, e.g. II (R5 = Me, Me2CH, cyclohexyl; R6 = H, Me2CH, Me2CHCH2) and oxazolone analogs. All these analogs were characterized by their "super" PPARα agonist activity and weak or partial agonist activity on PPARy in PPAR-GAL4 transactivation assays despite their similar binding affinities for both receptors. The cocrystal structures of II (R5 = Me; R6 = Me2CH) and rosiglitazone with PPARy-LBD were compared, and significant differences were found in their interactions with the receptor.

analogs in each subseries were further evaluated for in vivo efficacy. They all showed excellent anti-hyperglycemic efficacy in a db/db mouse model and hypolipidemic activity in hamster and dog models without provoking the typical PPAR γ -associated side effects in the rat tolerability assay.

IT 860780-59-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation of α -aryloxy-, α -benzoxazolidinyloxy- and α -benzisoxazolidinyloxy-substituted arylacetic acids as PPAR α/γ dual agonists with potent antihyperglycemic and lipid modulating activity)

RN 860780-59-2 HCAPLUS

CN Benzeneacetic acid, α -[4-[(dimethylamino)carbonyl]-2,6-dipropylphenoxy]- (9CI) (CA INDEX NAME)

REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:

2005:120912 HCAPLUS

DOCUMENT NUMBER:

142:218965

TITLE:

Preparation of alkynyl aryl carboxamides as

protein-tyrosine phosphatase (PTP) inhibitors

INVENTOR(S):

Swinnen, Dominique; Gerber, Patrick; Gonzalez, Jerome;

Bombrun, Agnes; Jorand-lebrun, Catherine

PATENT ASSIGNEE(S):

Applied Research Systems Ars Holding N.V., Neth.

Antilles

SOURCE:

PCT Int. Appl., 198 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT	KIND		DATE		APPLICATION NO.						DATE					
			-													
WO 2005012280				A1		20050210		1	WO 2004-EP51557					20040720		
₩:	ΑE,	AG,	AL,	AM,	ΑT,	ΑU,	ΑZ,	BA,	BB,	BG,	BR,	BW,	BY,	ΒZ,	CA,	CH,
	CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,
	GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	ΚP,	KR,	ΚZ,	LC,
	LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NI,
	NO,	NZ,	OM,	PG,	PH,	ΡL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,
	ТJ,	TM,	TN,	TR,	TT,	TZ,	UA,	ŪĠ,	US,	UZ,	VC,	VN,	YU,	ZA,	·ZM,	zw
RW:	BW,	GH,	GM,	ΚE,	LS,	MW,	ΜZ,	NA,	SD,	SL,	SZ,	TZ,	ŪĠ,	ZM,	ZW,	AM,
	AZ,	BY,	KG,	ΚZ,	MD,	RU,	ТJ,	TM,	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,
	EE,	ES,	FI,	FR,	GB,	GR,	ΗU,	ΙE,	IT,	LU,	MC,	NL,	PL,	PT,	RO,	SE,
	SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	ΝE,

SN, TD, TG AU 2004261400 AU 2004-261400 Α1 20050210 20040720 CA 2527861 AA CA 2004-2527861 20050210 20040720 EP 1654247 EP 2004-766274 Α1 20060510 20040720 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR PRIORITY APPLN. INFO.: EP 2003-102235 A 20030721 US 2003-517993P P 20031106 WO 2004-EP51557 W 20040720

OTHER SOURCE(S):

MARPAT 142:218965

GΙ

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [A = alkynyl, alkynylaryl, or alkynylheteroaryl; X = aryl, heteroaryl, cycloalkyl or heterocyclyl; X1 = (un)substituted aryl; n = 0 or 1; R1 and R2 independently = H or alkyl; R3 = alkyl, alkenyl, aryl, etc.; R4 and R5 = H, OH, F, alkyl, carboxy, etc.] and their pharmaceutically acceptable salt are prepared and disclosed as modulators of protein-tyrosine phosphatases (PTP). Thus, e.g., II was prepared via coupling of 4-bromobenzaldehyde with 1-decyne followed by reductive amination with 6-amino-2,2-dimethyl-4H-1,3-benzodioxin-4-one (preparation given), amidation with 3-cyclopentylpropanoyl chloride and deprotection. Tested compds. display an inhibition (IC50 values) with regard to PTP of preferably less than 20 µM, more preferred less than 5 µM. As PTP inhibitors, I should be useful for the treatment and/or prevention of an inflammatory disorder, obesity and/or metabolic disorders mediated by insulin resistance or hyperglycemia, comprising diabetes type I and/or II, inadequate glucose tolerance. insulin resistance, hyperlipidemia, hypertriglyceridemia- hypercholesterolemia, polycystic ovary syndrome (PCOS).

IT 843674-70-4P 843674-71-5P 843674-72-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of alkynyl aryl carboxamides as protein-tyrosine phosphatase (PTP) inhibitors)

RN 843674-70-4 HCAPLUS

CN Benzoic acid, 2-(carboxymethoxy)-5-[[[[4-(1-decynyl)phenyl]methyl][(2E)-1oxo-3-phenyl-2-propenyl]amino]methyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

HO₂C
$$CO_2H$$
 $C = C - (CH2)7$ Me

RN 843674-71-5 HCAPLUS

CNBenzoic acid, 2-(carboxymethoxy)-5-[[(3-cyclopentyl-1-oxopropyl)[[4-(1decynyl)phenyl]methyl]amino]methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me}-\text{ (CH}_2)_{7}-\text{C} & \text{C} \\ & & \text{CH}_2 \\ & & \text{CH}_2 \\ & & \text{CH}_2-\text{N}-\text{C}-\text{CH}_2-\text{CH}_2 \\ & & \text{HO}_2\text{C}-\text{CH}_2-\text{O} \\ & & \text{O} \end{array}$$

RN843674-72-6 HCAPLUS

CNBenzoic acid, 5-[[acetyl[[4-(1-decynyl)phenyl]methyl]amino]methyl]-2-(carboxymethoxy) - (9CI) (CA INDEX NAME)

Me-
$$(CH_2)_7$$
- C = C

AC

 CH_2 - N - CH_2 - CH_2 - CH_2 - CH_2 - CO_2H

REFERENCE COUNT:

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS 2 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

HCAPLUS COPYRIGHT 2006 ACS on STN ANSWER 10 OF 26

ACCESSION NUMBER:

2004:2833 HCAPLUS

DOCUMENT NUMBER:

140:77141

TITLE:

Preparation of 2-[4-(heteroarylaminomethyl)phenoxy]-2-

methylpropanoates for treating a hPPAR mediated

diseases

INVENTOR(S):

Dodic, Nerina; Dumaitre, Bernard Andre; Gellibert,

Francoise Jeanne; Sierra, Michael Lawrence

PATENT ASSIGNEE(S):

Smithkline Beecham Corporation, USA

SOURCE:

PCT Int. Appl., 89 pp.

DOCUMENT TYPE:

CODEN: PIXXD2

LANGUAGE:

Patent

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PAT	CENT :	NO.			KIN	D :	DATE			APPL	ICAT	ION 1	NO.		D.	ATE	
						-					- -				-		
WO	2004	0007	85		A2		2003	1231	1	WO 2	003-	EP64	17		2	0030	518
WO 2004000785 A3							2004	1014									
	W:	ΑE,	AG,	AL,	AM,	ΑT,	ΑU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,
		CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,
		GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KΕ,	KG,	KP,	KR,	ΚZ,	LC,	LK,	LR,
		LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NI,	NO.	NZ.	OM.

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PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT,
             TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
             FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     AU 2003237955
                          A1
                                 20040106
                                             AU 2003-237955
                                                                     20030618
     EP 1513796
                          A2
                                 20050316
                                             EP 2003-735642
                                                                     20030618
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
     JP 2005529965
                                 20051006
                                             JP 2004-514763
                          T2
                                                                     20030618
     US 2005222424
                          A1
                                 20051006
                                             US 2004-518347
                                                                     20041217
PRIORITY APPLN. INFO.:
                                             GB 2002-14139
                                                                     20020619
                                             WO 2003-EP6417
                                                                     20030618
```

OTHER SOURCE(S): MARPAT 140:77141 GI

The title compds. [I; R1, R2 = H, alkyl; R3, R4 = H, alkyl, OMe, CF, allyl, halo; n = 0-1; at least of X, Z and Y = O, S, N; R6 = alkyl, CF3, OMe, OCF3, halo; y = 0-5; R7 = H, CF3, alkyl (optionally substituted by phenyl), alkenyl with the proviso that when Z = S, O, R7 = H; R10 = H, alkyl; R5 = H, alkyl, alkoxyalkyl, alkenyl, alkoxy, etc.], useful for treatment of a hPPAR disease or condition such as dyslipidemia, syndrome X, heart failure, hypercholesterolemia, cardiovascular disease, diabetes, insulin resistance, hyperlipidemia, obesity, anorexia bulimia and anorexia nervosa (no biol. data given), were prepared Thus, reacting Et 2-(4-bromomethyl-2,6-dimethylphenoxy)-2-methylpropionate with [4-methyl-2-(4-trifluoromethylphenyl)thiazol-5-yl]thiophen-3-ylmethylamine (prepns. given) in the presence of cesium carbonate in 3-methyl-2-butanone followed by hydrolysis afforded II. Pharmaceutical composition comprising the compound I.

IT 639783-81-6P

RN 639783-90-7 HCAPLUS
CN Propanoic acid, 2-methyl-2-[2-methyl-4-[[[[4-methyl-2-[4-(trifluoromethyl)phenyl]-5-thiazolyl]methyl]-2-

propenylamino]methyl]phenoxy] - (9CI) (CA INDEX NAME)

F₃C

$$CH_2$$
 $N-CH_2-CH=CH_2$
 CH_2
 CH_2
 CH_2
 CH_2
 CH_2
 CH_2
 CH_2
 CH_2
 CH_2

RN 639783-92-9 HCAPLUS
CN Propanoic acid, 2-[4-[[(3-methoxypropyl)[[4-methyl-2-[4-(trifluoromethyl)phenyl]-5-thiazolyl]methyl]amino]methyl]-2-methylphenoxy]-2-methyl-(9CI) (CA INDEX NAME)

RN 639783-94-1 HCAPLUS
CN Propanoic acid, 2-[4-[[(2-furanylmethyl)[[4-methyl-2-[4-(trifluoromethyl)phenyl]-5-thiazolyl]methyl]amino]methyl]-2-methyl-(9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{HO}_2\text{C}-\text{C}-\text{O} \\ \text{Me} \\ \text{Me} \\ \text{Me} \\ \text{Me} \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{N} \\ \text{Me} \\ \\ \text{Me} \\ \end{array}$$

L4 ANSWER 11 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:

2004:2818 HCAPLUS

DOCUMENT NUMBER:

140:59406

TITLE:

Preparation of [[[(hetero)arylamino]methyl]phenoxy]ace tic acid derivatives as hPPAR activators for treatment

of cardiovascular disease and related disorders

INVENTOR(S):

Beswick, Paul John; Harling, John David; Kleanthous, Savvas; Patel, Vipulkumar Kantibhai; Simpson, Juliet

PATENT ASSIGNEE(S):

Smithkline Beecham Corporation, USA PCT Int. Appl., 98 pp.

SOURCE:

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

DOCUMENT TIPE

English

LANGUAGE:

1

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PA'	TENT	NO.			KIND DATE			APPLICATION NO.						DATE				
WO	2004	0007	62		A2	.2 20031231			WO 2003-EP6416					20030618				
WO	2004	004000762			A3 2		20041014											
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,	
		CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DΖ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	
		GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,	LK,	LR,	
		LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NI,	NO,	NZ,	OM,	
		PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	ТJ,	TM,	TN,	TR,	TT,	
		TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW						
	RW:	GH,	GM,	KΕ,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	ΑZ,	BY,	
		KG,	KZ,	MD,	RU,	TJ,	TM,	ΑT,	ΒE,	BG,	CH,	CY,	CZ,	DΕ,	DK,	EE,	ES,	
		FI,	FR,	GB,	GR,	HU,	ΙE,	ΙΤ,	LU,	MC,	NL,	PT,	RO,	SE,	SI,	SK,	TR,	
		BF,	ΒJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	ΝE,	SN,	TD,	TG	
CA	2489	359			AA		2003	1231	CA 2003-2489359					20030618				
ΑU	2003	2459	63		A1		2004	0106		AU 2003-245963					20030618			
EΡ	1513	795			A2		2005	0316		EP 2	003-	7380	57		20030618			
	R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,	
		ΙE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	AL,	TR,	BG,	CZ,	EE,	HU,	SK		
BR	2003	0119	35		Α		2005	0322		BR 2	003-1	1193	5		2	0030	618	
CN	1675	168			Α		2005	0928	CN 2003-819322					20030618				
JP 2005534673				T2	20051117			1	JP 2004-514762			20030618						

NO 2004005327 A 20050310 NO 2004-5327 20041203 US 2006074111 A1 20060406 US 2004-518778 20041217 PRIORITY APPLN. INFO.: GB 2002-14254 A 20020620 WO 2003-EP6416 W 20030618

OTHER SOURCE(S):

MARPAT 140:59406

GΙ

Title compds. I [wherein R1 and R2 = independently H or alkyl; X = a bond, CH2, or O; R3 and R4 = independently H, alkyl, OCH3, CF3, allyl, or halo; X1 = CH2, SO2, or CO; R5 = alkenyl, alkanoyl, alkylsulfonyl, or (un)substituted alkyl(phenyl); R6 = (un)substituted Ph or 6-membered heteroaryl; or pharmaceutically acceptable salts, solvates, or hydrolyzable esters thereof] were prepared as human peroxisome proliferator activated receptor (hPPAR) activators. For example, coupling of Et 2-methyl-2-[2-methyl-4-[[[4-(trifluoromethyl)benzyl]amino]methyl]phenoxy]p ropanoate with 2-bromo-6-[4-(trifluoromethyl)phenyl]pyridine in the presence of Pd(OAc)2, (R)-2,2'-bis(diphenylphosphino)-1,1'-binaphthyl, and cesium carbonate in toluene gave the tertiary amine. Saponification with NaOH in

ΙI

THF provided the acid II. Compds. of the invention showed at least 50% activation of hPPARO relative to the pos. control at concns. of 10-7 M or less. Thus, I and their pharmaceutical compns. are useful for the treatment of hPPAR mediated conditions, such as dyslipidemia, syndrome X, heart failure, hypercholesterolemia, cardiovascular disease, type II diabetes mellitus, type I diabetes, insulin resistance, hyperlipidemia, obesity, anorexia bulimia, or anorexia nervosa (no data). 637353-35-6P, [4-[[Butyl[4'-(trifluoromethyl)-1,1'-biphenyl-3-yl]amino]methyl]-2-methylphenoxy]acetic acid 637353-36-7P, [4-[(2-Methoxyethyl)[4'-(trifluoromethyl)-1,1'-biphenyl-3-

yl]amino]methyl]-2-methylphenoxy]acetic acid 637353-36-7P,
[4-[[(2-Methoxyethyl) [4'-(trifluoromethyl)-1,1'-biphenyl-3yl]amino]methyl]-2-methylphenoxy]acetic acid 637353-37-8P,
[2-Methyl-4-[[(pentyl) [4'-(trifluoromethyl)-1,1'-biphenyl-3yl]amino]methyl]phenoxy]acetic acid 637353-38-9P,
[4-[[(2-Cyclopropylethyl) [4'-(trifluoromethyl)-1,1'-biphenyl-3yl]amino]methyl]-2-methylphenoxy]acetic acid 637353-39-0P,
[2-Methyl-4-[[propyl[4'-(trifluoromethyl)-1,1'-biphenyl-3yl]amino]methyl]phenoxy]acetic acid 637353-40-3P,

IT

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[2-Methyl-4-[[[2-(methylthio)ethyl][4'-(trifluoromethyl)-1,1'-biphenyl-3-
yl]amino]methyl]phenoxy]acetic acid 637353-41-4P,
[4-[[Butyl[2-methyl-4'-(trifluoromethyl)-1,1'-biphenyl-3-yl]amino]methyl]-
2-methylphenoxy]acetic acid 637353-42-5P, [4-[[(2-
Methoxyethyl) [2-methyl-4'-(trifluoromethyl)-1,1'-biphenyl-3-
yl]amino]methyl]-2-methylphenoxy]acetic acid 637353-43-6P,
[4-[[(Butyryl)[4'-(trifluoromethyl)-1,1'-biphenyl-3-yl]amino]methyl]-2-
methylphenoxy]acetic acid 637353-44-7P, [2-Methyl-4-
[[(propylsulfonyl)[4'-(trifluoromethyl)-1,1'-biphenyl-3-
yl]amino]methyl]phenoxy]acetic acid 637353-45-8P,
[4-[[Butyl[4'-(trifluoromethyl)-1,1'-biphenyl-3-yl]amino]sulfonyl]-2-
methylphenoxy]acetic acid 637353-46-9P, [2-Methyl-4-
[[(pentyl)[4'-(trifluoromethyl)-1,1'-biphenyl-3-
yl]amino]sulfonyl]phenoxy]acetic acid 637353-47-0P,
[4-[[(2-Cyclopropylethyl)[4'-(trifluoromethyl)-1,1'-biphenyl-3-
yl]amino]sulfonyl]-2-methylphenoxy]acetic acid 637353-56-1P,
[4-[Butyl(2,4'-dimethyl-1,1'-biphenyl-3-yl)amino]methyl]-2-
methylphenoxy]acetic acid 637353-57-2P, [4-[[Butyl(4'-fluoro-2-
methyl-1,1'-biphenyl-3-yl)amino]methyl]-2-methylphenoxy]acetic acid
637353-58-3P, [4-[[Butyl(4'-cyano-2-methyl-1,1'-biphenyl-3-
yl)amino]methyl]-2-methylphenoxy]acetic acid 637353-59-4P,
[4-[[Butyl(4'-methoxy-2-methyl-1,1'-biphenyl-3-yl)amino]methyl]-2-
methylphenoxy]acetic acid 637353-60-7P, [4-[[Butyl(4'-chloro-2-
methyl-1,1'-biphenyl-3-yl)amino]methyl]-2-methylphenoxy]acetic acid
637353-61-8P, [4-[[(4'-Chloro-2-methyl-1,1'-biphenyl-3-yl)(2-
methoxyethyl)amino]methyl]-2-methylphenoxy]acetic acid
637353-62-9P, [4-[[(2,4'-Dimethyl-1,1'-biphenyl-3-yl)(2-
methoxyethyl)amino]methyl]-2-methylphenoxy]acetic acid
637353-63-0P, [4-[[(2-Methoxyethyl)(4'-methoxy-2-methyl-1,1'-
biphenyl-3-yl)amino]methyl]-2-methylphenoxy]acetic acid
637353-64-1P, [2-Methyl-4-[[[2-methyl-4'-(trifluoromethyl)-1,1'-
biphenyl-3-yl] (propyl) amino] methyl] phenoxy] acetic acid
637353-65-2P, [4-[[(4'-Chloro-2-methyl-1,1'-biphenyl-3-
yl)(propyl)amino]methyl]-2-methylphenoxy]acetic acid 637353-66-3P
, [4-[[(2,4'-Dimethyl-1,1'-biphenyl-3-yl)(propyl)amino]methyl]-2-
methylphenoxy]acetic acid 637353-67-4P, [4-[[(4'-Fluoro-2-methyl-
1,1'-biphenyl-3-yl) (propyl) amino] methyl]-2-methylphenoxy] acetic acid
637353-68-5P, [4-[[(4'-Cyano-2-methyl-1,1'-biphenyl-3-
yl)(propyl)amino]methyl]-2-methylphenoxy]acetic acid 637353-69-6P
, [4-[[(4'-Methoxy-2-methyl-1,1'-biphenyl-3-yl)(propyl)amino]methyl]-2-
methylphenoxy]acetic acid 637353-84-5P, [4-[[Butyl[2-methyl-4'-
(trifluoromethyl) -1,1'-biphenyl-3-yl]amino]sulfonyl]-2-
methylphenoxy]acetic acid
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
   (hPPAR activator; preparation of [[[(hetero)arylamino]methyl]phenoxy]acetic
   acid derivs. as hPPAR activators for treatment of cardiovascular
   disease and related disorders)
637353-35-6 HCAPLUS
Acetic acid, [4-[[butyl[4'-(trifluoromethyl)[1,1'-biphenyl]-3-
yl]amino]methyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)
```

RN CN

$$r_3$$
C r_2 r_3 C r_4 r_5 r_6 r_6 r_6 r_6 r_6 r_7 r_8 $r_$

RN 637353-36-7 HCAPLUS

CN Acetic acid, [4-[[(2-methoxyethyl)[4'-(trifluoromethyl)[1,1'-biphenyl]-3-yl]amino]methyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{F}_3\text{C} & \text{CH}_2\text{--}\text{CH}_2\text{--}\text{OMe} \\ \hline & \text{N}\text{---}\text{R} \end{array}$$

RN 637353-37-8 HCAPLUS

CN Acetic acid, [2-methyl-4-[[pentyl[4'-(trifluoromethyl)[1,1'-biphenyl]-3-yl]amino]methyl]phenoxy]- (9CI) (CA INDEX NAME)

$$Me - (CH_2)_4$$
 $N - CH_2$
 $O - CH_2 - CO_2H$

RN 637353-38-9 HCAPLUS

CN Acetic acid, [4-[[(2-cyclopropylethyl) [4'-(trifluoromethyl) [1,1'-biphenyl]-3-yl]amino]methyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

$$CH_2$$
 CH_2
 CH_2

RN 637353-39-0 HCAPLUS

CN Acetic acid, [2-methyl-4-[[propyl[4'-(trifluoromethyl)[1,1'-biphenyl]-3-yl]amino]methyl]phenoxy]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} & \text{O-CH}_2\text{-CO}_2\text{H} \\ \hline & \text{N-CH}_2 & \text{O-CH}_2\text{-CO}_2\text{H} \\ \end{array}$$

RN 637353-40-3 HCAPLUS

CN Acetic acid, [2-methyl-4-[[[2-(methylthio)ethyl][4'-(trifluoromethyl)[1,1'-biphenyl]-3-yl]amino]methyl]phenoxy]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{CH}_2-\text{CH}_2-\text{SMe} \\ \\ \text{N}-\text{R} \end{array}$$

$$\begin{array}{c} \text{Me} \\ \text{O-} \text{CH}_2\text{--}\text{CO}_2\text{H} \\ \\ \text{R-} \text{CH}_2 \end{array}$$

RN 637353-41-4 HCAPLUS

CN Acetic acid, [4-[[butyl[2-methyl-4'-(trifluoromethyl)[1,1'-biphenyl]-3-yl]amino]methyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

$$Me$$
 $N-CH_2$
 $N-CH_2$
 $N-CH_2$
 $N-CH_2$

RN 637353-42-5 HCAPLUS

CN Acetic acid, [4-[[(2-methoxyethyl)[2-methyl-4'-(trifluoromethyl)[1,1'-biphenyl]-3-yl]amino]methyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

RN 637353-43-6 HCAPLUS

CN Acetic acid, [2-methyl-4-[[(1-oxobutyl)[4'-(trifluoromethyl)[1,1'-biphenyl]-3-yl]amino]methyl]phenoxy]- (9CI) (CA INDEX NAME)

RN 637353-44-7 HCAPLUS

CN Acetic acid, [2-methyl-4-[[(propylsulfonyl) [4'-(trifluoromethyl) [1,1'-biphenyl]-3-yl]amino]methyl]phenoxy]- (9CI) (CA INDEX NAME)

RN 637353-45-8 HCAPLUS

CN Acetic acid, [4-[[butyl[4'-(trifluoromethyl)[1,1'-biphenyl]-3-yl]amino]sulfonyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

RN 637353-46-9 HCAPLUS

CN Acetic acid, [2-methyl-4-[[pentyl[4'-(trifluoromethyl)[1,1'-biphenyl]-3-yl]amino]sulfonyl]phenoxy]- (9CI) (CA INDEX NAME)

RN 637353-47-0 HCAPLUS

CN Acetic acid, [4-[[(2-cyclopropylethyl) [4'-(trifluoromethyl) [1,1'-biphenyl]-3-yl]amino]sulfonyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

$$HO_2C-CH_2-O$$
 Me
 $O=S=O$
 CH_2-CH_2-N
 CF_3

RN 637353-56-1 HCAPLUS

CN Acetic acid, [4-[[butyl(2,4'-dimethyl[1,1'-biphenyl]-3-yl)amino]methyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

Me
$$n-Bu$$
 $O-CH_2-CO_2H$

RN 637353-57-2 HCAPLUS

CN Acetic acid, [4-[[butyl(4'-fluoro-2-methyl[1,1'-biphenyl]-3-yl)amino]methyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} & \text{N-Bu} & \text{O-CH}_2\text{-CO}_2\text{H} \\ \hline & \text{N-CH}_2 & \text{O-CH}_2\text{-CO}_2\text{H} \\ \end{array}$$

RN 637353-58-3 HCAPLUS

CN Acetic acid, [4-[[butyl(4'-cyano-2-methyl[1,1'-biphenyl]-3-yl)amino]methyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

RN 637353-59-4 HCAPLUS

CN Acetic acid, [4-[[butyl(4'-methoxy-2-methyl[1,1'-biphenyl]-3-yl)amino]methyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{Me} & \text{O-CH}_2\text{-CO}_2\text{H} \\ \hline & \text{N-CH}_2 & \text{O-CH}_2\text{-CO}_2\text{H} \\ \end{array}$$

RN 637353-60-7 HCAPLUS

CN Acetic acid, [4-[[butyl(4'-chloro-2-methyl[1,1'-biphenyl]-3-yl)amino]methyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{N-CH}_2 \end{array} \qquad \begin{array}{c} \text{Me} \\ \text{O-CH}_2 - \text{CO}_2 \text{H} \end{array}$$

RN 637353-61-8 HCAPLUS

CN Acetic acid, [4-[[(4'-chloro-2-methyl[1,1'-biphenyl]-3-yl)(2-methoxyethyl)amino]methyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Cl} & \text{Me} & \text{CH}_2\text{--}\text{CH}_2\text{--}\text{OMe} \\ & \text{N}\text{---}\text{R} \end{array}$$

RN 637353-62-9 HCAPLUS

CN Acetic acid, [4-[[(2,4'-dimethyl[1,1'-biphenyl]-3-yl)(2-methoxyethyl)amino]methyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

RN 637353-63-0 HCAPLUS

CN Acetic acid, [4-[[(2-methoxyethyl)(4'-methoxy-2-methyl[1,1'-biphenyl]-3-yl)amino]methyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

RN 637353-64-1 HCAPLUS

CN Acetic acid, [2-methyl-4-[[[2-methyl-4'-(trifluoromethyl)[1,1'-biphenyl]-3-yl]propylamino]methyl]phenoxy]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{N-Pr} \\ \hline & \text{N-CH}_2 \\ \end{array}$$

RN 637353-65-2 HCAPLUS

CN Acetic acid, [4-[[(4'-chloro-2-methyl[1,1'-biphenyl]-3-yl)propylamino]methyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

C1 Me
$$n-Pr$$
 $N-CH_2$ O- CH_2-CO_2H

RN 637353-66-3 HCAPLUS

CN Acetic acid, [4-[[(2,4'-dimethyl[1,1'-biphenyl]-3-yl)propylamino]methyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

Me
$$n-Pr$$
 $N-CH_2$ $O-CH_2-CO_2H$

RN 637353-67-4 HCAPLUS

Updated Search

CN Acetic acid, [4-[[(4'-fluoro-2-methyl[1,1'-biphenyl]-3-yl)propylamino]methyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

RN 637353-68-5 HCAPLUS

CN Acetic acid, [4-[[(4'-cyano-2-methyl[1,1'-biphenyl]-3-yl)propylamino]methyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{NC} \\ \text{Me} \\ \text{n-Pr} \\ \text{N-CH}_2 \\ \end{array}$$

RN 637353-69-6 HCAPLUS

CN Acetic acid, [4-[[(4'-methoxy-2-methyl[1,1'-biphenyl]-3-yl)propylamino]methyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

MeO Me
$$n-Pr$$
 $N-CH_2$ $O-CH_2-CO_2H$

RN 637353-84-5 HCAPLUS

CN Acetic acid, [4-[[butyl[2-methyl-4'-(trifluoromethyl)[1,1'-biphenyl]-3-yl]amino]sulfonyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

L4 ANSWER 12 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2

2003:696736 HCAPLUS

DOCUMENT NUMBER:

139:230769

TITLE:

Preparation of (arylalkyl)thiazoles and oxazoles as peroxisome proliferator activated receptor modulators for treating diabetes mellitus and atherosclerosis Conner, Scott Eugene; Mantlo, Nathan Bryan; Zhu,

INVENTOR(S):

Guoxin Eli Lilly and Company, USA

PCT Int. Appl., 153 pp. CODEN: PIXXD2

DOCUMENT TYPE:

Patent English

LANGUAGE:

SOURCE:

Eng

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT ASSIGNEE(S):

Pi	PATENT NO.					KIND DATE				APPLICATION NO.					DATE			
W	WO 2003072102					A1 20030904			WO 2003-US2680					20030213				
		W:	ΑE,	ΑG,	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,
			CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,
			GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	ΚP,	KR,	ΚZ,	LC,	LK,	LR,
			LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	OM,	PH,
			PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	ТJ,	TM,	TN,	TR,	TT,	TZ,
			UA,	UG,	US,	UΖ,	VC,	VN,	ΥU,	ZA,	ZM,	zw						
		RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	ŪĠ,	ZM,	ZW,	AM,	AZ,	BY,
								TM,										
			FI,	FR,	GB,	GR,	HU,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	SI,	SK,	TR,	BF,
								GΑ,										•
Α	J 2	20032				A1		2003									00302	213
E	P 1	4806	542			A1		2004	1201	I	EP 20	003-1	71078	30		20	00302	213
		R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,
			ΙE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	AL,	TR,	BG,	CZ,	EE,	HU,	SK	
J1	P 2	20055	2834	16		Т2		2005	922	į	JP 20	003-5	57084	18		2	00302	213
US	S 2	20060	8466	53		A1		20060	0420	τ	JS 20	004-5	50510	03		2	0408	317
PRIORI	ΓY	APPI	N. 3	INFO	. :					US 2002-359807P)7P	P 20020225			
										V	NO 20	J-800	JS268	30	Ţ	v 20	00302	213
OMITTED (201	TD 07	(~)				~~											

OTHER SOURCE(S):

MARPAT 139:230769

GI

$$\begin{array}{c|c}
R8 & & & & \\
R7 & & & & \\
R7 & & & & \\
R6 & & & & \\
\end{array}$$

$$F_3C$$
 N N Me OH OH OH

AB Title compds. I [wherein R3 = H or alkoxy; R4 = H or alkyl; R5 = alkyl, alkenyl, or (un) substituted aryl(oxy) alkyl or arylthioalkyl; R6 = CF3, OCF3, (hydroxy)alkyl, alkylcarbamoyl, carboxyalkoxy, or (un)substituted aryloxy, arylthio, pyridinyl, pyrimidinyl, pyrazinyl, or arylalkyl; R7 and R8 = independently H, CF3, or alkyl; R9 and R10 = independently H, alkyl, alkenyl, or alkoxy; T1 = C or N; Q = bond, O, O(CH2)q, or C; q = 1-2; W = constant = 1O, S, SO2, NHSO2, etc.; X = CmH2m; m = 0-2; Y and Z = independently O, N,or S wherein at least 1 of Y and Z = O or S; A = CO2H, alkylnitrile, CONH2, or (CH2)nCO2R19; n = 0-3; R19 = H or (un)substituted alkyl or arylmethyl; and pharmaceutically acceptable salts thereof] were prepared as peroxisome proliferator activated receptor (PPAR) agonists (no data). For example, (4-mercapto-2-methylphenoxy) acetic acid Et ester was coupled with 5-chloromethyl-4-phenethyl-2-(4-trifluoromethylphenyl)thiazole in the presence of Cs2CO3 in MeCN to give the (phenylthiomethyl)thiazole (83.5%), which was saponified with LiOH in THF to provide II. I and their pharmaceutical compns. are useful for the prevention and or treatment of diabetes mellitus and atherosclerosis (no data).

Ι

IT 592519-34-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(PPAR agonist; preparation of PPAR agonists for treating diabetes mellitus and atherosclerosis)

RN 592519-34-1 HCAPLUS

CN Benzenepropanoic acid, 4-[[bis[[4-methyl-2-[4-(trifluoromethyl)phenyl]-5-thiazolyl]methyl]amino]methyl]-2-methyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 592519-33-0 CMF C35 H31 F6 N3 O2 S2

CM 2

CRN 76-05-1 CMF C2 H F3 O2

REFERENCE COUNT:

THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 13 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:

2003:696734 HCAPLUS

DOCUMENT NUMBER:

139:230768

TITLE:

Preparation of (arylalkyl)thiazoles and oxazoles as peroxisome proliferator activated receptor modulators

for treating diabetes mellitus, syndrome X, and

cardiovascular disease

INVENTOR(S):

Conner, Scott Eugene; Knobelsdorf, James Allen; Mantlo, Nathan Bryan; Schkeryantz, Jeffrey Michael; Shen, Quanrong; Warshawsky, Alan M.; Zhu, Guoxin

PATENT ASSIGNEE(S):

Eli Lilly and Company, USA

SOURCE:

PCT Int. Appl., 223 pp. CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.		KIND	DATE	APPLICATION NO.	DATE
WO 200307210	0	A1	20030904	WO 2003-US2679	20030213
W: AE,	AG, AL,	AM, AT	, AU, AZ,	BA, BB, BG, BR, BY,	BZ, CA, CH, CN,
CO,	CR, CU,	CZ, DE	, DK, DM,	DZ, EC, EE, ES, FI,	GB, GD, GE, GH,
GM,	HR, HU,	ID, IL	, IN, IS,	JP, KE, KG, KP, KR,	KZ, LC, LK, LR,
LS,	LT, LU,	LV, MA	, MD, MG,	MK, MN, MW, MX, MZ,	NO, NZ, OM, PH,
PL,	PT, RO,	RU, SC	, SD, SE,	SG, SK, SL, TJ, TM,	TN, TR, TT, TZ,

UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG AU 2003217274 AU 2003-217274 A1 20030909 20030213 EP 1480640 **A1** 20041201 EP 2003-713316 20030213 AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK US 2005107449 20050519 US 2003-505089 A1 20030213 JP 2005529077 **T2** 20050929 JP 2003-570846 20030213 PRIORITY APPLN. INFO.: US 2002-359808P 20020225 WO 2003-US2679 20030213

Ι

OTHER SOURCE(S):

MARPAT 139:230768

GI

Title compds. I [wherein R3, R4, R30, and R40= independently H, alkyl, AB halo, or alkoxy; R5 = (un)substituted alkyl, alkenyl, aryl(oxy)alkyl, or arylthioalkyl; or when R5 = alkyl, R5 may be combined with W to form a heterocycloalkyl fused to the oxazole or thiazole ring; R6 = trihalomethyl, trihalomethoxy, (hydroxy)alkyl, alkylcarbamoyl, tetramethyldioxaborolanyl, halo, alkanoyl, carboxyalkoxy, (cyclo)alkoxy, tetrahydropyranyloxy, morpholinyl, or (un)substituted aryloxy, arylthio, heterocyclyloxy, pyridinyl, pyrimidinyl, pyrazinyl, or arylalkyl; R7 and R8 = independently H, CF3, or alkyl; R9 = (un)substituted (aryl)alkyl or alkenyl; R10 = H or alkyl; Q = a bond, O, or CH2; T1 = C or N; W = CH2, O, OCH2, S, SO2, or (un) substituted CONH, NH, or NHCH2; X = C, CH2C, or CCH2; Y and Z = independently O, N, or S wherein at least 1 of Y and <math>Z = O or S; A = CO2H, alkylnitrile, CONH2, or (CH2)nCO2R19; n = 0-3; R19 = H or alkyl; and pharmaceutically acceptable salts thereof] were prepared as peroxisome proliferator activated receptor δ (PPAR δ) modulators (no data). For example, (4-mercapto-2-methylphenoxy) acetic acid Et ester was

condensed with 1-[4-[2-(2-chloro-6-fluorophenyl)ethyl]-2-(4-trifluoromethylphenyl)thiazol-5-yl]ethanol in the presence of PBu3 and 1,1'-(azodicarbonyl)bipiperidine in toluene. Deesterification with LiOH in THF produced II. I and their pharmaceutical compns. are useful for the prevention and or treatment of diabetes mellitus, syndrome X, and cardiovascular disease (no data).

IT 591777-10-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(PPAR modulator; preparation of PPAR modulators for treating diabetes mellitus, syndrome X, and cardiovascular disease)

RN 591777-10-5 HCAPLUS

Benzenepropanoic acid, 2-methyl-4-[[methyl[2-[4-(1-methylethyl)-2-[4-(trifluoromethyl)phenyl]-5-thiazolyl]propyl]amino]methyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CN

CRN 591777-09-2 CMF C28 H33 F3 N2 O2 S

CM 2

CRN 76-05-1 CMF C2 H F3 O2

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 14 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:335066 HCAPLUS

DOCUMENT NUMBER: 138:353734

TITLE: Preparation of phenoxyacetic acids as modulators of

 $\delta\text{-peroxisome}$ proliferator-activated receptors (PPAR- δ) for the treatment of dyslipidemia and

coronary cardiac diseases

INVENTOR(S): Bischoff, Hilmar; Dittrich-Wengenroth, Elke; Heckroth,

Heike; Vaupel, Andrea; Woltering, Michael; Weigand,

Stefan

PATENT ASSIGNEE(S): Bayer Aktiengesellschaft, Germany

SOURCE:

PCT Int. Appl., 97 pp.

CODEN: PIXXD2

DOCUMENT TYPE: LANGUAGE: Patent German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PA	KIND DATE			APPLICATION NO.					DATE								
						_									-		
WO	2003	0356	03		A1		2003	0501		WO 2	002-1	EP11:	275		2	0021	009
	W:	ΑE,	AG,	AL,	AM,	ΑT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,
		CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FΙ,	GB,	GD,	GE,	GH,
		GM,	HR,	HU,	ID,	IL,	IN,	ıs,	JP,	ΚE,	KG,	ΚP,	KR,	ΚZ,	LC,	LK,	LR,
		LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	ΜZ,	NO,	ΝZ,	OM,	PH,
		PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	ТJ,	TM,	TN,	TR,	TT,	TZ,
		UA,	UG,	US,	UΖ,	VC,	VN,	YU,	ZA,	ZM,	ZW						
	RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	ŪĠ,	ZM,	ZW,	AM,	ΑZ,	BY,
											CH,						
		FI,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	SK,	TR,	BF,	ВJ,	CF,
		CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG			
DE	1015	1390			A1		2003	0508		DE 2	001-	1015	1390		2	0011	018
CA	2463	226			AA		2003	0501		CA 2	002-2	2463	226		2	0021	009
EP	1438	285			A1		2004	0721		EP 2	002-	7772	95		2	0021	009
	R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,
		ΙE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	AL,	TR,	ВG,	CZ,	EE,	SK		
JP	2005	5063	79		T2		2005	0303		JP 2	003-	5381	19		2	0021	009
US	2005	1540	51		A1		2005	0714		US 2	003-4	1927	61		2	0021	009
PRIORIT	Y APP	LN.	INFO	. :						DE 2	001-	1015	1390		A 2	0011	018
										WO 2	002-1	EP11:	275	1	₩ 2	0021	009
OTHER SOURCE(S):					MARI	PAT	138:	3537	34								

THER SOURCE (S): PARPAL 130:35373

GΙ

AB Title compds. I [A = CH2, CH2CH2; X = 0, S, CH2; R1, R2, R3 = H, alkyl, cycloalkyl, etc.; R4 = H, alkyl; R5, R6 = H, oxo; R7 = H, alkyl; R8 = alky, (CH2)nE; E = (un)substituted cycloalkyl, e.g., alkyl, CF3, OH, etc.; n = 1-2; R9, R10 = H, alkyl, alkoxy, etc.; R11, R12 = H, alkyl; R13 = H, hydrolyzable group (sic)] and their pharmaceutically acceptable salts were prepared For example, coupling of cyclohexylamine II, e.g., prepared from 4-hydroxy-3-methylbenzaldehyde in 2-steps, and 2-bromo-N-(2,4-dichlorophenyl)acetamide, followed by ester hydrolysis afforded phenoxyacetic acid III. In dose response studies on PPARδ-GAL4 chimeric receptors, the EC50 values of 7-examples of I ranged from 1-100 nM. The invention discloses the preparation of novel substituted acetic acid derivs., e.g., fibrates, for their use as potent compds. of PPAR-δ activation. Compds. I are claimed as medicaments for the treatment of dyslipidemia and coronary cardiac diseases.

III

IT 518336-74-8P 518336-75-9P 518336-76-0P
518336-78-2P 518336-86-2P 518336-88-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
 (Uses)

(drug candidate; preparation of phenoxyacetic acids as modulators of PPAR delta for the treatment of dyslipidemia and coronary cardiac diseases) 518336-74-8 HCAPLUS

CN Propanoic acid, 2-[4-[[(cyclopropylmethyl)[2-[(2,4-difluorophenyl)amino]-2-oxoethyl]amino]methyl]-2-methylphenoxy]-2-methyl- (9CI) (CA INDEX NAME)

RN

RN 518336-75-9 HCAPLUS

CN Propanoic acid, 2-[4-[[(cyclopropylmethyl)[2-[(2,4-dichlorophenyl)amino]-2-oxoethyl]amino]methyl]-2-methylphenoxy]-2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & &$$

RN 518336-76-0 HCAPLUS

CN Propanoic acid, 2-[4-[[[2-[(2,4-difluorophenyl)amino]-2-oxoethyl]heptylamino]methyl]-2-methylphenoxy]-2-methyl- (9CI) (CA INDEX NAME)

RN 518336-78-2 HCAPLUS

CN Propanoic acid, 2-[4-[[[2-[(2,4-dichlorophenyl)amino]-2-oxoethyl]pentylamino]methyl]-2-methylphenoxy]-2-methyl- (9CI) (CA INDEX NAME)

RN 518336-86-2 HCAPLUS

CN Propanoic acid, 2-[4-[[(cyclohexylmethyl) [2-[(2,4-dichlorophenyl)amino]-2-oxoethyl]amino]methyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ \text{Me} & & & \\ & & & \\ \text{HO}_2\text{C}-\text{CH}-\text{O} & \\ & & & \\ \text{Me} & & \\ \end{array}$$

RN 518336-88-4 HCAPLUS

CN Propanoic acid, 2-[4-[[(cyclohexylmethyl) [2-[(2,4-dichlorophenyl)amino]-2-oxoethyl]amino]methyl]-2-methylphenoxy]-2-methyl- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 15 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1985:95418 HCAPLUS

DOCUMENT NUMBER:

102:95418

TITLE:

2-(Dimethylamino)ethyl [methyl(dimethylsulfamoyl)pheno

xy]acetates

INVENTOR(S):

Oniscu, Cornelia; Nitelea, Ion; Botez, Gheorghe;

Stanescu, Cornelia

PATENT ASSIGNEE(S):

Institutul de Cercetari Chimico-Farmaceutice, Rom.

SOURCE:

Rom., 2 pp. CODEN: RUXXA3

DOCUMENT TYPE:

Patent Romanian

LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
				-	
RO 77264	В	19810817	RO 1978-94788		19780726
ORITY APPLN. INFO.:			RO 1978-94788	Α	19780726

PRIC OTHER SOURCE(S):

CASREACT 102:95418

GI

AB Esters I (R = H, Me), which were prepared, are useful as central nervous system stimulants (no data). Thus, 2,4-Me(Me2NSO2)C6H3OCH2CO2H was converted to its acid chloride, and the latter was treated with Me2NCH2CH2OH to give the appropriate I (R = H).

Ι

IT 29148-99-0 94882-99-2

> RL: RCT (Reactant); RACT (Reactant or reagent) (esterification of, by ethanolamine derivative)

RN29148-99-0 HCAPLUS

CN Acetic acid, [4-[(dimethylamino)sulfonyl]-2,5-dimethylphenoxy]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & & \\ \text{Me} & & & & \\ & & & \\ & & & \\ & & & \\ \text{HO}_2\text{C-CH}_2\text{-O} & & & \\ & & & \\ & & & \\ \text{Me} & & \\ \end{array}$$

RN94882-99-2 HCAPLUS

CNAcetic acid, [4-[(dimethylamino)sulfonyl]-2,6-dimethylphenoxy]- (9CI)

$$Me_{2}N-S$$

$$Me_{2}N-S$$

$$Me_{3}N-S$$

$$Me_{4}N-S$$

IT 29148-95-6

RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with thionyl chloride)

RN 29148-95-6 HCAPLUS

CN Acetic acid, [4-[(dimethylamino)sulfonyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & \\ \hline \\ S-NMe_2 \\ \hline \\ Me \\ O-CH_2-CO_2H \end{array}$$

L4 ANSWER 16 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:

1984:530416 HCAPLUS

DOCUMENT NUMBER:

101:130416

TITLE:

(Dimethylamino) ethyl esters of 2-(sulfamoylphenoxy) propionic acids

INVENTOR(S):

Oniscu, Corneliu; Bibian Cilianu, Stefan; Dobrescu, Dumitru; Chirita, Mihai; Szekeli, Zoltan; Murgu, Lucia

PATENT ASSIGNEE(S):

Institutul de Cercetari Chimico-Farmaceutice, Rom.

SOURCE:

Rom., 3 pp.

DOCUMENT TYPE:

CODEN: RUXXA3

LANGUAGE:

Patent Romanian

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
RO 82051	В	19830707	RO 1981-104368	19810522
PRIORITY APPLN. INFO.:			RO 1981-104368	19810522
OTHER SOURCE(S):	CASREA	CT 101:13041	.6	

GI

AB Esters I (R = H, Me; R1 = H, Cl, Me, OMe) were prepared, and they are useful as central nervous system stimulants (no data). Thus, 4,2-Cl(Me2NSO2)C6H3OCHMeCO2H was treated with SOCl2 and Me2NCH2CH2OH to give 4,2-Cl(Me2NSO2)C6H3OCHMeCO2CH2CH2NMe2.

IT 49816-52-6 91859-24-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(esterification of, by thionyl chloride and ethanolamine derivative)

Ι

RN 49816-52-6 HCAPLUS
CN Propanoic acid, 2-[4-[(dimethylamino)sulfonyl]-2-methylphenoxy]- (9CI)
(CA INDEX NAME)

RN 91859-24-4 HCAPLUS
CN Propanoic acid, 2-[4-[(dimethylamino)sulfonyl]-3-methylphenoxy]- (9CI)
(CA INDEX NAME)

L4 ANSWER 17 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1983:483603 HCAPLUS

DOCUMENT NUMBER: 99:83603

TITLE:

Laboratory screening tests of systemic and chemotherapeutic fungicidal activity of some

aryloxyalkanecarboxylic acid derivatives

AUTHOR (S):

Stec, Maria; Eckstein, Zygmunt

CORPORATE SOURCE: SOURCE:

Inst. Org. Chem. Technol., Tech. Univ., Warsaw, Pol. Acta Phytopathologica Academiae Scientiarum Hungaricae

(1982), 17(1-2), 179-91

CODEN: APYPBZ; ISSN: 0001-6780

DOCUMENT TYPE:

Journal English

LANGUAGE:

GΙ

OCH2CO2Et II, R=H, R1=CH=CHNO2 III, $R=CH=CHNO_2$, $R^1=H$

$$C1$$
 $OCH_2CONHOH$ $C1$ IV

Of 66 compds. of the general formula AroCH(R)COX (I; R = H or Me; X = AB HNOH, OMe, OEt, or OH; Ar = 1-naphthalenyl and substituted phenyls), those having the 2-nitrovinyl toxophor on the phenoxyacetic acid moiety, especially in

positions 3 or 4, were the most effective against Phytophthora infestans on the 3 apical leaves of tomato. The sulfanamide and hydrazide toxophors on phenoxyacetic or (\pm) -2-phenoxypropionic acid derivs. also were highly effective. Mevin (II) [24602-89-9], Pavin (III) [24634-65-9], 2,4,6-TH (IV) [13370-24-6], and I; R = H, X = HNOH, Ar = C10H7-(1) [13370-51-9] also showed protective and systemic activity on potatoes. Most of 20 compds. effective against Alternaria tenuis and Venturia inaequalis in vitro, contained 1,3-dioxacyclane and 2-nitrovinyl groups.

IT 27455-81-8 49816-52-6 RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses)

(fungicidal activity of)

27455-81-8 HCAPLUS RN

Propanoic acid, 2-[4-[(dimethylamino)sulfonyl]-2,5-dimethylphenoxy]- (9CI) CN (CA INDEX NAME)

L4 ANSWER 18 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1975:156014 HCAPLUS

DOCUMENT NUMBER: 82:156014

TITLE: Chromanones derived from β -cresoxypropionic acids

AUTHOR(S): Cocarla, I.; Mazilu, I.; Nicu, M.; Botez, Gh.

CORPORATE SOURCE: Inst. Politeh., Iasi, Rom.

SOURCE: Buletinul Institutului Politehnic din Iasi, Sectia 2:

Chimie (1973), 19(1-2), 83-9 CODEN: BICMCF; ISSN: 0373-3246

DOCUMENT TYPE: Journal

LANGUAGE: Romanian

GI For diagram(s), see printed CA Issue.

AB Chromones I (R = Me, R1 = SO2NMe2, SO2NEt2) were prepared by chlorosulfonylating 2-MeC6H4OCH2CO2Et, aminating 2,4-

Me(ClSO2)C6H3OCH2CH2CO2Et, hydrolyzing 2,4-Me(R1)C6H3OCH2CO2Et, and cyclizing the acids with PCl5-AlCl3. I (R = SO2NMe2, SO2NEt2, R1 = Me)

were similarly prepared from 4-MeC6H4OCH2CH2CO2Et.

IT 55654-57-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and cyclization of)

RN 55654-57-4 HCAPLUS

CN Propanoic acid, 3-[4-[(diethylamino)sulfonyl]-2-methylphenoxy]- (9CI) (CA

INDEX NAME)

IT 55654-55-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and hydrolysis of)

RN 55654-55-2 HCAPLUS

CN Propanoic acid, 3-[4-[(dimethylamino)sulfonyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

L4 ANSWER 19 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1973:545506 HCAPLUS

DOCUMENT NUMBER: 79:145506

TITLE: Nuclear magnetic resonance spectra of derivatives of

aryloxyalkyl carboxylic sulfonamides. II. NMR spectra of sulfonamides of α -phenoxypropionic

and α -phenoxybutyric acids Oniscu, Corneliu; Botez, Gh.

AUTHOR(S): Oniscu, Corneliu; Botez, Gh CORPORATE SOURCE: Inst. Politeh., Iasi, Rom.

SOURCE: Buletinul Institutului Politehnic din Iasi (1972),

18(3-4), 119-23

CODEN: BUPIAE; ISSN: 0032-6100

DOCUMENT TYPE: Journal LANGUAGE: Romanian

GI For diagram(s), see printed CA Issue.

AB The NMR spectra of 42 sulfonamides (I, R = Me, Et; R1 = OH, OEt, NHNH2; R2 = OH, NH2, NMe2, NEt2, morpholino; R3, R4 = H, C1, Me, OMe, Me2CH) derived

from α -phenoxypropionic and α -phenoxybutyric acids were

recorded at 60 MHz in Me2SO-d6 and analyzed. The spectra supported the assigned structures. When R2 = NH2 the sulfonamidic protons gave a

singlet due to rapid exchange.

IT 49816-52-6

RL: PRP (Properties)

(NMR of)

RN49816-52-6 HCAPLUS

Propanoic acid, 2-[4-[(dimethylamino)sulfonyl]-2-methylphenoxy]- (9CI) CN (CA INDEX NAME)

ANSWER 20 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:

1973:498944 HCAPLUS

DOCUMENT NUMBER:

79:98944

Journal

TITLE:

Nuclear magnetic resonance spectra of

aminosulfonylphenoxyacetatesBotez, Gh.; Oniscu, Corneliu

AUTHOR(S): CORPORATE SOURCE:

Inst. Politeh., Iasi, Rom.

SOURCE:

Buletinul Institutului Politehnic din Iasi (1972),

18(3-4), 107-12

CODEN: BUPIAE; ISSN: 0032-6100

DOCUMENT TYPE:

LANGUAGE: Romanian

AB The NMR of 38 derivs. of aminosulfonylphenoxyacetic acids, amides, and hydrazides with various substituents on the amine and on the benzene ring

are reported. IT 49816-52-6

RL: PRP (Properties)

(NMR of)

RN 49816-52-6 HCAPLUS

CN Propanoic acid, 2-[4-[(dimethylamino)sulfonyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

ANSWER 21 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN

1972:405106 HCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 77:5106

Monoethanolaminosulfonyl-, diethanolaminosulfonyl- and TITLE:

morpholinosulfonyl-phenoxyacetic derivatives

AUTHOR (S): Oniscu, Corneliu; Gorea, Camelia; Merica, Ecaterina;

Botez, Gh.

CORPORATE SOURCE: Inst. Politeh., Iasi, Rom.

SOURCE: Buletinul Institutului Politehnic din Iasi (1971),

14 (3-4), 101-14

CODEN: BUPIAE; ISSN: 0032-6100

DOCUMENT TYPE:

Journal

LANGUAGE: Romanian

Treatment of (methylphenoxy) acetic acids with EtOH and H2SO4 at 78° gave rate consts. which were a function of the position of the Me group (2 > 4 > 3). Reaction of Et (methylphenoxy)acetates or (methylphenoxy)acetic hydrazides with HSO3Cl gave the sulfochlorides. Reaction of the sulfochlorides with monoethanolamine, diethanolamine, or morpholine gave

23 sulfonamides.

36685-71-9P 36685-82-2P 36691-82-4P IT

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN36685-71-9 HCAPLUS

Acetic acid, [4-[[bis(2-hydroxyethyl)amino]sulfonyl]-3-methylphenoxy]-CN (CA INDEX NAME)

RN 36685-82-2 HCAPLUS

Acetic acid, [4-[[bis(2-hydroxyethyl)amino]sulfonyl]-2,5-dimethylphenoxy]-CN (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{O} & \text{CH}_2-\text{CH}_2-\text{OH} \\ \parallel & \parallel \\ \text{S-N-CH}_2-\text{CH}_2-\text{OH} \\ \parallel & \text{O} \\ \text{HO}_2\text{C-CH}_2-\text{O} \end{array}$$

RN 36691-82-4 HCAPLUS

CNAcetic acid, [4-[[bis(2-hydroxyethyl)amino]sulfonyl]-2-methylphenoxy]-(9CI) (CA INDEX NAME)

L4 ANSWER 22 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1971:498288 HCAPLUS

DOCUMENT NUMBER: 75:98288

TITLE: Phenoxybutyric acid sulfamides. I. Sulfamide

derivatives of the α -phenoxy-, α -cresoxy-,

and α -xylenoxybutyric acids

AUTHOR(S): Botez, Gh.; Gorea, Camelia; Oniscu, Corneliu; Merica,

Ecaterina

CORPORATE SOURCE: Dep. Org. Ind., Polytech. Inst., Iasi, Rom.

SOURCE: Buletinul Institutului Politehnic din Iasi (1970),

16(1-2), 161-72

CODEN: BUPIAE; ISSN: 0032-6100

DOCUMENT TYPE: Journal LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB Sulfamide derivs. (58) of α -phenoxy-(I), α -cresoxy-, and α -(xylyloxy)-butyric acids were prepared to study their hypocholesterolemic effects. The Et ester of I reacted with excess ClSO3H

to give p-(ClO2S)C6H4OCH(Et)CO2Et, which reacted with NH3 in Me2CO to give Et α -(4-sulfamoylphenoxy)butyrate (II), with Me2NH to yield the N,N-dimethyl analog and with morpholine to give the morpholino analog. All esters on alkaline hydrolysis gave the free acids. II with NH2NH2 gave α -(p-sulfamoylphenoxy)-butyric acid hydrazide. Chlorosulfonation of Et α -(2-methylphenoxy)butyrate began at 3-9°, and ended at 15° to yield the 4-sulfamoyl derivative, which was converted into III [R = H, Me, Et, or (NR2 =) morpholino; R1 = H, Et, NHNH2; R2 = Me; R3 = R1 = H]. Similarly prepared were the III (R2 = R4 = H, R3 = Me), III (R2 = R3

= Me, R4 = H), III (R2 = R4 = Me, R3 = H), IV (R2 = R3 = H), IV (R2 = H, R3 = Me), and IV (R2 = Me, R3 = H) analogs.

IT 33491-38-2P 33491-41-7P 33491-42-8P 33491-55-3P 33491-65-5P 33491-66-6P

33602-19-6P 33815-06-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 33491-38-2 HCAPLUS

CN Butyric acid, 2-[[4-(dimethylsulfamoyl)-o-tolyl]oxy]- (8CI) (CA INDEX NAME)

RN 33491-41-7 HCAPLUS
CN Butyric acid, 2-[[4-(dimethylsulfamoyl)-m-tolyl]oxy]- (8CI) (CA INDEX NAME)

RN 33491-42-8 HCAPLUS
CN Butyric acid, 2-[[4-(diethylsulfamoyl)-m-tolyl]oxy]- (8CI) (CA INDEX NAME)

RN 33491-55-3 HCAPLUS CN Butyric acid, 2-[[4-(diethylsulfamoyl)-2,3-xylyl]oxy]- (8CI) (CA INDEX NAME)

RN 33491-65-5 HCAPLUS

CN Butyric acid, 2-[[4-(dimethylsulfamoyl)-2,5-xylyl]oxy]- (8CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & \\ & & & & & \\ \text{Me} & & & & \\ & & & & \\ \text{CO}_2\text{H} & & & & \\ & & & & \\ \text{Et-CH-O} & & & & \\ & & & & \\ \end{array}$$

RN 33491-66-6 HCAPLUS

CN Butyric acid, 2-[[4-(diethylsulfamoyl)-2,5-xylyl]oxy]- (8CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \circ \\ & \parallel \\ \text{S-NEt}_2 \\ & \parallel \\ \text{Et-CH-O} \end{array}$$

RN 33602-19-6 HCAPLUS

CN Butyric acid, 2-[[4-(diethylsulfamoyl)-o-tolyl]oxy]- (8CI) (CA INDEX NAME)

33815-06-4 HCAPLUS RN

Butyric acid, 2-[[4-(dimethylsulfamoyl)-2,3-xylyl]oxy]- (8CI) CN (CA INDEX

ANSWER 23 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN L4

ACCESSION NUMBER: 1971:141206 HCAPLUS

DOCUMENT NUMBER: 74:141206

TITLE: Phenoxypropionic acid sulfonamides. II.

Sulfonamidated derivatives of α -cresoxypropionic

 α -xylyloxypropionic acids

AUTHOR(S): Botez, Gh.; Gorea, Camelia; Merica, Ecaterina; Oniscu,

Corneliu

CORPORATE SOURCE: Inst. Politeh., Iasi, Rom.

SOURCE: Buletinul Institutului Politehnic din Iasi (1969),

15(1-2), 67-78

CODEN: BUPIAE; ISSN: 0032-6100

DOCUMENT TYPE: Journal LANGUAGE: Romanian

Potential plant growth regulators (38) were synthesized by treating Et α -cresoxypropionate and Et α -xylyloxypropionate with HSO3Cl

(1:7, 15-40°); the chlorosulfonate derivs. were treated with NH3 or

NHEt2 to form the corresponding sulfonamides, which, by alkaline hydrolysis gave the title compds. The hydrazides of the α -cresoxy and

α-xylyloxypropionic acids were also prepared.

31640-01-4P 31649-53-3P 31776-67-7P IT

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 31640-01-4 HCAPLUS

CN Propionic acid, 2-[[4-(diethylsulfamoyl)-m-tolyl]oxy]- (8CI) (CA INDEX NAME)

RN 31649-53-3 HCAPLUS

CN Propionic acid, 2-[[4-(diethylsulfamoyl)-3,5-xylyl]oxy]- (8CI) (CA INDEX NAME)

RN 31776-67-7 HCAPLUS

CN Propionic acid, 2-[[4-(diethylsulfamoyl)-2,5-xylyl]oxy]- (8CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ \text{Me} & & & \\ & & & \\ \text{Me} & & & \\ & & & \\ \text{HO}_2\text{C}-\text{CH}-\text{O} & & \\ & & & \\ \end{array}$$

L4 ANSWER 24 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1970:520246 HCAPLUS

DOCUMENT NUMBER: 73:120246

TITLE: Preparation and properties of some derivatives of

sulfamylphenoxyacetic acid

AUTHOR(S): Eckstein, Zygmunt; Rusek, Dorota; Cudnoch, Stanislawa;

Arct, Jacek

CORPORATE SOURCE: Zakl. Technol. Srodkow Ochr. Roslin, Politech.

Warszaw., Warsaw, Pol.

SOURCE: Przemysl Chemiczny (1970), 49(6), 341-5

CODEN: PRCHAB; ISSN: 0033-2496

DOCUMENT TYPE: Journal LANGUAGE: Polish

GI For diagram(s), see printed CA Issue.

AB Esters of the title compds. (I, Y = sulfonyl, alkylsulfamoyl or

alkylaminosulfamoyl) were prepared from I (R = alkyl, Y = H, X = H, halogen

or alkyl) by treatment with ClSO3H at 0-40° and then with NH3, amines or hydrazine. Thus I (R = Me, Y = SO2NHEt-4, X = H) (Ia) and 30 other I were prepared Ia was hydrolyzed with 5% NaOH to give I (R = X = H, Y = SO2NHEt-4) (II). Similarly prepared were 9 II analogs. I and II were screened for mycostatic action and elongation of plant cells.

IT 29148-95-6P 29148-99-0P

RN 29148-95-6 HCAPLUS

CN Acetic acid, [4-[(dimethylamino)sulfonyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

RN 29148-99-0 HCAPLUS

CN Acetic acid, [4-[(dimethylamino)sulfonyl]-2,5-dimethylphenoxy]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & \\ & & & & \\ \text{Me} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ &$$

L4 ANSWER 25 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1970:434965 HCAPLUS

DOCUMENT NUMBER: 73:34965

TITLE: Preparation and properties of some derivatives of

(+-)-2-(sulfamylaryloxy)-propionic acid

AUTHOR(S): Krassowska, Barbara; Ejmocki, Zdzislaw; Eckstein,

Zygmunt

CORPORATE SOURCE: Politech. Warszawskiej, Warsaw, Pol.

SOURCE: Przemysl Chemiczny (1970), 49(4), 218-22

CODEN: PRCHAB; ISSN: 0033-2496

DOCUMENT TYPE: Journal

LANGUAGE: Polish

AB Preparation of derivs. of racemic 2-aryloxyalkanecarboxylic acids, substituted in o- or p-position with a sulfamoyl, N-alkyl, or N-methoxysulfamoyl group are described. The compds. in question are of the general formula: R1R2NSO2ArOCHMeCO2Me. The starting materials for their synthesis were several racemic 2-aryloxypropionic acids [ArOCHMeCO2H], obtained by condensation of 1-cyanoethyl benzenesulfonate [PhS(O)2OCH(CN)Me] with phenol, 2-methyl-, 2,5-dimethyl-4-chloro-3-methyl-, or 2,5-dichlorophenol,

and with 1-naphthol. All of the above 2-aryloxypropionic acids were esterified with MeOH (70-90% yields), the Me esters were dissolved in CHCl3 and treated with ClSO2OH, and the resulting crude sulfonyl chlorides were reacted (in Me2CO or C6H6 solution) with NH3, N-methyl-, N-methoxy-, or N,N-dimethylamine. The yields, m.ps., and the characteristic ir absorption bands of the various Me esters [ArOCHMeCO2Me] and free acids [ArOCHMeCO2H] prepared by the authors are tabulated. The substituents in the aromatic nucleus were chosen in order to maximize fungicidal activity and minimize plant growth regulatory effects. The compds. showed good systematic fungicidal activity against Phytophthora infestans and were effective in treating tomatoes infected with this pathogen.

IT 27455-81-8P 49816-52-6P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of) RN 27455-81-8 HCAPLUS

CN Propanoic acid, 2-[4-[(dimethylamino)sulfonyl]-2,5-dimethylphenoxy]- (9CI) (CA INDEX NAME)

RN 49816-52-6 HCAPLUS
CN Propanoic acid, 2-[4-[(dimethylamino)sulfonyl]-2-methylphenoxy]- (9CI)
(CA INDEX NAME)

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STRUCTURE UPLOADED L1

L2 0 S L1

L3 197 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 14:03:46 ON 21 AUG 2006

26 S L3

1 S L4 AND BESWICK, P?/AU L5

L6 25 S L4 NOT L5

L7 0 S L6 AND HARLING, J?/AU L8

0 S L6 AND KLEANTHOUS, S?/AU

L9 0 S L6 AND LAMBERT, M?/AU

0 S L6 AND KANTIBHAI, V?/AU L10

L11 0 S L6 AND SIMPSON, J?/AU

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=> s 13

L4

L12 1 L3

=> d l12, all, 1

ANSWER 1 OF 1 CAOLD COPYRIGHT 2006 ACS on STN L12

AΝ CA60:6834d CAOLD

TТ sulfonamides of phenoxyacetic acids - (III) imidazoline derivs. from sulfonamido compds. of phenoxyacetic acid and of cresoxyacetic acids and their hypotensive activity

Botez, Gh.; Enescu, L. ΑU

- 10518778

IT 25841-44-5 50283-86-8 90872-23-4 91013-73-9 91248-66-7 91248-67-8 92147-57-4 92491-64-0 93568-52-6 93568-53-7 93568-54-8 94025-11-3 94266-90-7 95295-63-9 96636-15-6

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=> S 25841-44-5/RN

L13 1 25841-44-5/RN

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=> D L13 SQIDE 1-

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L13 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN

RN 25841-44-5 REGISTRY

CN Benzenesulfonamide, 4-[(4,5-dihydro-1H-imidazol-2-yl)methoxy]-2-methyl-(9CI) (CA INDEX NAME)

. 10518778

OTHER CA INDEX NAMES:

CN o-Toluenesulfonamide, 4-(2-imidazolin-2-ylmethoxy)- (7CI, 8CI)

OTHER NAMES:

CN 2-(4-Sulfamoyl-3-methyl-phenoxymethyl)-2-imidazoline

FS 3D CONCORD

MF C11 H15 N3 O3 S

CI COM

LC STN Files: CA, CAOLD, CAPLUS, TOXCENTER

DT.CA CAplus document type: Journal

RL.NP Roles from non-patents: BIOL (Biological study); NORL (No role in record)

$$\begin{array}{c|c}
H \\
N \\
\longrightarrow CH_2 - O \\
\longrightarrow N \\
\longrightarrow S - NH_2 \\
\longrightarrow Me O
\end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 2 REFERENCES IN FILE CA (1907 TO DATE)
- 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- 2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

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	ENTRY	SESSION
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TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

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=> S 93568-53-7/RN

L14 1 93568-53-7/RN

=> SET NOTICE 1 DISPLAY

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=> D L14 SQIDE 1-

YOU HAVE REQUESTED DATA FROM 1 ANSWERS - CONTINUE? Y/(N):Y THE ESTIMATED COST FOR THIS REQUEST IS 6.36 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:Y

L14 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN

RN 93568-53-7 REGISTRY

CN Acetic acid, [[4-(diethylsulfamoyl)-m-tolyl]oxy]- (7CI) (CA INDEX NAME)

FS 3D CONCORD

MF C13 H19 N O5 S

LC STN Files: CA, CAOLD, CAPLUS

DT.CA CAplus document type: Journal

RL.NP Roles from non-patents: NORL (No role in record)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- 1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> SET NOTICE LOGIN DISPLAY

NOTICE SET TO OFF FOR DISPLAY COMMAND SET COMMAND COMPLETED

=>

=> FIL REGISTRY

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 2.34 334.39 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE -19.50 0.00

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STRUCTURE FILE UPDATES: 20 AUG 2006 HIGHEST RN 902860-89-3 DICTIONARY FILE UPDATES: 20 AUG 2006 HIGHEST RN 902860-89-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=> S 93568-54-8/RN

L15 1 93568-54-8/RN

=> SET NOTICE 1 DISPLAY

NOTICE SET TO 1 U.S. DOLLAR FOR DISPLAY COMMAND SET COMMAND COMPLETED

=> D L15 SQIDE 1-

YOU HAVE REQUESTED DATA FROM 1 ANSWERS - CONTINUE? Y/(N):y THE ESTIMATED COST FOR THIS REQUEST IS 6.36 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L15 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN
RN 93568-54-8 REGISTRY
CN Acetic acid, [[4-(diethylsulfamoyl)-o-tolyl]oxy]- (7CI) (CA INDEX NAME)

FS 3D CONCORD

MF C13 H19 N O5 S

STN Files: CA, CAOLD, CAPLUS

DT.CA CAplus document type: Journal

RL.NP Roles from non-patents: NORL (No role in record)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- 1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> SET NOTICE LOGIN DISPLAY

NOTICE SET TO OFF FOR DISPLAY COMMAND SET COMMAND COMPLETED

= >

=> FIL REGISTRY

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	2.34	336.73
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-19.50

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STRUCTURE FILE UPDATES: 20 AUG 2006 HIGHEST RN 902860-89-3 DICTIONARY FILE UPDATES: 20 AUG 2006 HIGHEST RN 902860-89-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=> S 50283-86-8/RN

L16 1 50283-86-8/RN

=> SET NOTICE 1 DISPLAY

NOTICE SET TO 1 U.S. DOLLAR FOR DISPLAY COMMAND SET COMMAND COMPLETED

=> D L16 SQIDE 1-

YOU HAVE REQUESTED DATA FROM 1 ANSWERS - CONTINUE? Y/(N):Y THE ESTIMATED COST FOR THIS REQUEST IS 6.36 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:Y

L16 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN

RN 50283-86-8 REGISTRY

CN Acetic acid, [4-[(diethylamino)sulfonyl]phenoxy]- (9CI) (CA INDEX NAME) OTHER CA INDEX NAMES:

CN Acetic acid, [p-(diethylsulfamoyl)phenoxy] - (6CI, 7CI)

FS 3D CONCORD

MF C12 H17 N O5 S

CI COM

LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CHEMCATS, TOXCENTER (*File contains numerically searchable property data)

DT.CA CAplus document type: Journal

RL.NP Roles from non-patents: BIOL (Biological study); PRP (Properties); NORL (No role in record)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 5 REFERENCES IN FILE CA (1907 TO DATE)
- 5 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- 2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> SET NOTICE LOGIN DISPLAY

- 10518778

NOTICE SET TO OFF FOR DISPLAY COMMAND SET COMMAND COMPLETED

=>

=> FIL REGISTRY

CA SUBSCRIBER PRICE

COST IN U.S. DOLLARS

SINCE FILE TOTAL
ENTRY SESSION
2.34 339.07

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL
ENTRY SESSION

0.00

-19.50

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STRUCTURE FILE UPDATES: 20 AUG 2006 HIGHEST RN 902860-89-3 DICTIONARY FILE UPDATES: 20 AUG 2006 HIGHEST RN 902860-89-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=> S 91248-67-8/RN

L17 1 91248-67-8/RN

=> SET NOTICE 1 DISPLAY

NOTICE SET TO 1 U.S. DOLLAR FOR DISPLAY COMMAND SET COMMAND COMPLETED

=> D L17 SQIDE 1-

YOU HAVE REQUESTED DATA FROM 1 ANSWERS - CONTINUE? Y/(N):Y THE ESTIMATED COST FOR THIS REQUEST IS 6.36 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:Y

L17 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN

RN 91248-67-8 REGISTRY

CN Acetic acid, [(4-sulfamoyl-o-tolyl)oxy]-, ethyl ester (7CI) (CA INDEX NAME)

FS 3D CONCORD

MF C11 H15 N O5 S

LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS

(*File contains numerically searchable property data)

DT.CA CAplus document type: Journal

RL.NP Roles from non-patents: NORL (No role in record)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 2 REFERENCES IN FILE CA (1907 TO DATE)
- 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- 2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> SET NOTICE LOGIN DISPLAY

NOTICE SET TO OFF FOR DISPLAY COMMAND SET COMMAND COMPLETED

=>

=> FIL REGISTRY

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	3.22	342.29
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-19.50

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STRUCTURE FILE UPDATES: 20 AUG 2006 HIGHEST RN 902860-89-3 DICTIONARY FILE UPDATES: 20 AUG 2006 HIGHEST RN 902860-89-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Updated Search

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=> S 94025-11-3/RN

L18 1 94025-11-3/RN

=> SET NOTICE 1 DISPLAY

NOTICE SET TO 1 U.S. DOLLAR FOR DISPLAY COMMAND SET COMMAND COMPLETED

=> D L18 SQIDE 1-

YOU HAVE REQUESTED DATA FROM 1 ANSWERS - CONTINUE? Y/(N):Y THE ESTIMATED COST FOR THIS REQUEST IS 6.36 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:Y

L18 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN

RN 94025-11-3 REGISTRY

CN Acetic acid, [p-(diethylsulfamoyl)phenoxy]-, ethyl ester (7CI) (CA INDEX NAME)

FS 3D CONCORD

MF C14 H21 N O5 S

LC STN Files: CA, CAOLD, CAPLUS

DT.CA CAplus document type: Journal

RL.NP Roles from non-patents: NORL (No role in record)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 2 REFERENCES IN FILE CA (1907 TO DATE)
- 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)
- 2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> SET NOTICE LOGIN DISPLAY

NOTICE SET TO OFF FOR DISPLAY COMMAND SET COMMAND COMPLETED

• 10518778

= ;